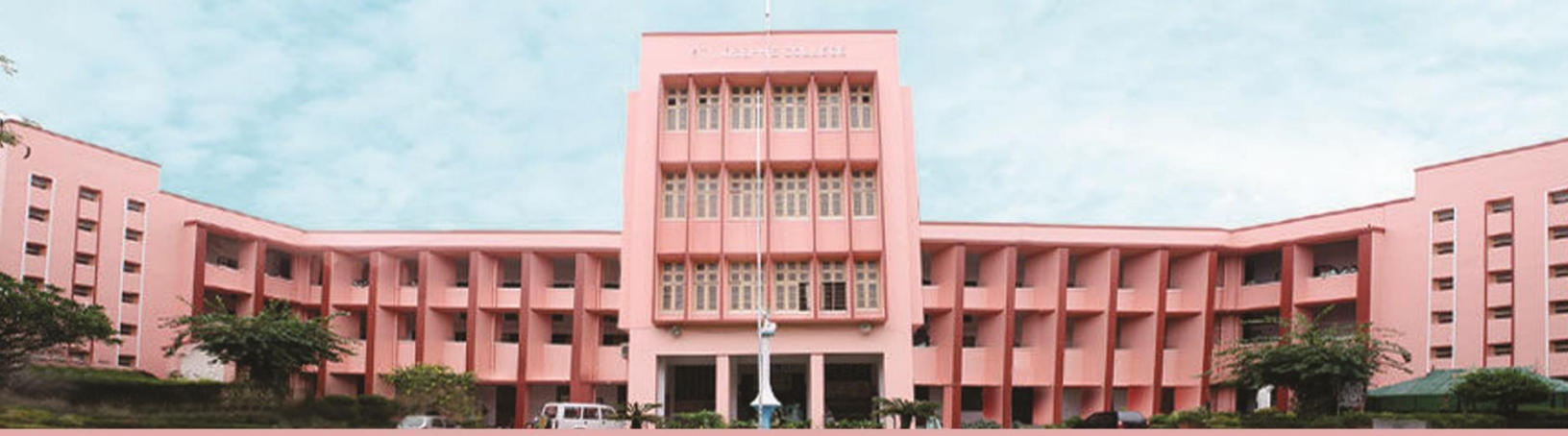

ST. JOSEPH'S COLLEGE (AUTONOMOUS)

IRINJALAKUDA

CURRICULA AND SYLLABI FOR

MSC CHEMISTRY

Under Choice Based Credit & Semester System

2020 Admissions

St. Joseph's College (Autonomous), Irinjalakuda

Department of Chemistry

Board of Studies in 2019

Name, designation and address of BOS members

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FOREWORD

The future of the credibility of the higher education system depends on the success of the implementation of autonomy. The anticipated outcome of the whole exercise depends, in particular, on the mainstay of any educational institution- the curricular aspects. As an autonomous college since 2016, St. Joseph's has the mandate to visualize appropriate curricula for particular programmes, update and revise them periodically, and make sure that the expected outcomes are successfully achieved.

A wide range of course options that are in tune with the emerging national and global trends ad relevant to the local needs were considered by the institution prior to the P.G. restructuring exercise. Diversity and flexibility, career orientation, skill acquisition, and research enhancement were considered and a structured feedback system established to gather the opinions and suggestions of all the stakeholders including the students, the faculty, the staff, the industry experts, the alumnae, the parents and the employers.

Curricula evolved also took into account the attainment of program, program specific and course outcomes. Evaluation of the curricular intake and delivery is done at the year end to find suggestions for change.I sincerely acknowledge the members on the various Boards of Studies and on the Academic Council for their time and expertise in helping us come to a decision regarding Curricula and Syllabi restructuring and redesigning. Thanks are also due to the team IQAC for their relentless endeavours in enhancing quality of education delivery, and in particular, for their efforts to organize workshops and invited talks to orient the faculty and students towards the necessities implied in the restructuring process. I would also like to thank the Heads of Departments and faculty and staff who co-operated with the same.

Principal

ACKNOWLEDGEMENT

I acknowledge with gratitude all the guidance and help given by our Principal, Dr. Sr. Isabel during the course of restructuring of the syllabi. I also remember and acknowledge with gratitude all the members of the Board of Studies (Chemistry) for their constructive suggestions and contributions in restructuring the syllabi of all the courses in Chemistry. I am also grateful to all the members of the Curriculum Committee of the college for their guidance during the syllabus restructuring process. Above all, I bow my head before God Almighty for all the guidance he has continuously given to us all our endeavours.

Dr. Deena Antony C
Associate Professor & Head
Department of Chemistry

CONTENT

St. Joseph's College, (Autonomous), Irinjalakuda

Department of Chemistry

(2020 Admission)

Preface

Science education is central to the development of any society. This can be achieved only by revamping the undergraduate programme to make it effective and meaningful. The development of scientific temper in society necessitates proper education and guidance. In order to achieve this, one must update the developments in the field of science. An effective science education can be imparted at the undergraduate level only by revamping the present curriculum. To achieve this goal, the curriculum should be restructured by emphasizing various aspects such as the creativity of students, knowledge of current developments in the discipline, awareness of environmental impacts due to the development of science and technology, and the skills essential for handling equipment and instruments in laboratories and industries.

Chemistry, being an experimental science, demands testing theories through practical laboratory experiences for a thorough understanding of the subject. Nowadays, chemistry laboratories in academic institutions use large amounts of chemicals. The awareness and implementation of eco-friendly experiments becomes a global necessity. It is essential to ensure that laboratory chemicals are used at a minimal level without affecting the skill and understanding aimed through laboratory sessions. This creates an environmental awareness among the students and pollution free atmosphere in the campus.

During the preparation of the syllabus, the existing syllabus, UGC model curriculum and the syllabi of other universities have been referred. Care has been taken to ensure that the syllabus is compatible with the syllabi of other universities at the same level. Sufficient emphasis is given in the syllabus for training in laboratory skills and instrumentation.

The units of the syllabus are well defined. A list of references and further readings are provided at the end of each unit.

St. Joseph's College, (Autonomous), Irinjalakuda

STUDENT ATTRIBUTES

The motto of the institution is "Light, Life, and Love"
Light for the illumination of the heart and mind
Life for the fullness of growth – physical, mental, intellectual and spiritual
Love for fellowship with the Supreme & with one another
The motto enshrines the vision of the Founders for the students and constitutes the foundation for the acquisition of the following student attributes envisioned by the institution.

- Empowerment
- Life Long Learning
- Holistic Development
- Value Orientation
- Social Responsibility
- Nation Building Capacity
- Green Thinking
- Creativity & Innovation
- Acquiring Life Skills
- Discipline
- Leadership / Team skills
- Problem solving skills
- Communicability

The above Student Attributes will be attained in the span of their student life at St. Joseph's College through various activities such as

- Curricular, Co-curricular & extra-curricular
- Sports, games, fine arts and cultural
- Enrichment / certificate courses
- Extension / outreach programmes
- Healthy / Best practices

PROGRAMME OUTCOMES

At the end of a postgraduate programme, the student would have:

1. Acquired the ability for critical thinking and problem solving
2. Attained life skills and communication skills
3. Inculcated moral and ethical values
4. Become a promoter of unpolluted environs and proactive society
5. Developed a culture of research and lifelong learning
6. Become an empowered woman aware of global perspectives and national realities

PROGRAMME SPECIFIC OUTCOME

	Program Specific Outcomes
PSO1	To develop skills in the proper handling of instruments and chemicals
PSO2	To be exposed to the different processes used in industries and their applications
PSO3	To develop the ability for applying the principles of chemistry

AIMS AND OBJECTIVES

First Semester

- To understand how quantum mechanics is applied, starting from simple systems to hydrogen / like atom/s.
- To understand the basic principles of bonding, nuclear and nanochemistry and periodic table.
- To understand the basic principles of structure and bonding in organic chemistry, conformational analysis and stereochemistry.
- To understand the basic principles of irreversible thermodynamics.
- To understand the higher level facts and concepts in chemical kinetics and catalysis.

Second Semester

- To understand how group theory is applied in molecular spectroscopy and in chemical bonding
- To understand the basic and higher level concept in coordination chemistry
- To identify the mechanism of organic chemical reactions, including pericyclic and photochemical reactions.
- To understand the basic and higher level concepts in electrochemistry, solid state chemistry and statistical thermodynamics.

Third Semester

- To understand the basic and higher level concepts in various spectroscopy.
- To understand the basic and higher level concepts in organometallic chemistry and bioinorganic chemistry.
- To understand the basic concepts in oxidation reduction rearrangement reactions in organic chemistry.
- To understand various strategy used in synthetic organic chemistry.

- To know the basics of multistep synthesis and retrosynthetic analysis.

Fourth Semester

- To understand the principle, working and application of various analyticalinstruments.
- To understand the basic principles of catalysis, synthesis of different catalyst, deactivation of catalyst.
- To understand classification and properties of ceramic, nano and composite materials.
- To understand the basic and higher level concepts in organometallic chemistry.

COURSE DESIGN

The MSc Chemistry programme includes

i. Core courses
ii. Elective Courses
iii. Project Work / Dissertation
iv. Comprehensive Viva-voce
v. Audit Courses

The MSc Chemistry programme contains 18 compulsory Core courses, 3 Elective Courses, 1 Project Work / Dissertation, 1 Comprehensive Viva-voce and 2 Audit Courses. No course carries more than 4 credits. The student can select any Choice based elective course offered by the department which offers the core courses, depending on the availability of teachers and infrastructure facilities, in the institution.

Duration of the programme

The minimum duration for completion of a four semester PG programme is two years. The maximum period for completion is four years. The duration of each semester will be 90 working days, inclusive of examinations, spread over five months. Odd semesters will be held from June to October and even semesters from November to March subject to the academic calendar of St. Joseph's College (Autonomous), Irinjalakuda.

Programme structure

The MSc Chemistry programme includes three types of courses: Core courses, Elective courses and Audit Courses. Project Work and Comprehensive Viva-voce are mandatory for all regular programmes and these shall be done in the end semester. Total credit for the MSc Chemistry programme is 80 (eighty), this describes the weightage of the

course concerned and the pattern of distribution is as detailed below:

Programme Duration	Four Semesters
Core courses	18
Elective Courses	3
Project Work / Dissertation	1
Comprehensive Viva-voce	1
Minimum attendance required	>70%

Elective courses shall be spread over either in the Third & Fourth Semesters combined or in any one of these Semesters (III / IV). Study Tour / Field visit / Industrial visit / Trip for specimen collection may be conducted as a part of the Programme.

Semester	Course Title	Suggested Area
I	Ability Enhancement Course (AEC)	Internship / Seminar presentation / Publications / Case study analysis / Industrial or Practical Training/Community linkage programme /Book reviews etc.
II	Professional Competency Course (PCC)	To test the skill level of students like testing the application level of different software such as SPSS/R/ Econometrics / Pythan/any software relevant to the programme of study / Translations etc.

Courses and Credit distribution

The required number of credits as specified in the syllabus/regulations must be acquired by the student to qualify for the degree. A student shall accumulate a minimum of 80 credits for the successful completion of the MSc Chemistry programmes.

Semester	Course	Teaching Hours	Credit
I	Core Courses (Theory/Practical)	*234*	*16*
II	Core Courses (Theory/Practical)	*216*	*21*
III	Core Courses (Theory/Practical) Elective Courses (Theory/Practical)	234	*12* *4*
IV	Core Courses (Theory / Practical) Including: • Comprehensive Viva-voce (Optional) • Project Work / Dissertation Elective Courses (Theory/ Practical)	*216*	*13* *2* *48*
Total credit			***80***

Audit Courses:

In addition to the above courses there will be two Audit Courses *(Ability Enhancement Course & Professional Competency Course)* with 4 credits each. The college will conduct examinations for these courses in respective semesters and intimate /upload the results of the same to the Controller of Examinations of St. Joseph's College (Autonomous) Irinjalakuda. The College will intimate/upload the results of the same to the University on the stipulated date during the third semester. The credits will not be counted for evaluating the overall SGPA & CGPA. The details of Audit courses are given below.

Semester	Course	Teaching Hours	Credit

I	***Audit Course I :*** *Ability Enhancement Course (AEC)*	*Total teaching hours*	*4*
II	***Audit Course II :*** *Professional Competency Course (PCC)*	*Total teaching hours*	*4*

Project Work / Dissertation & Comprehensive Viva-Voce

There is a Project work with dissertation and Comprehensive Viva-Voce as separate courses relating to the core area under study in the end Semester and included in the Core Courses. Viva-voce related to Project work is one of the criteria for Project Work evaluation. Students have to submit a Project Report / Dissertation in the prescribed structure and format as a part of the Project Work undertaken. There will be external and internal evaluation for Project Work/ Comprehensive Viva-Voce and these shall be combined in the proportion of 4:1.

COURSE CODE FORMAT

The following are the common guidelines for coding various courses in order to get a uniform identification. It is advisable to assign a nine Digit Code (combination of Alpha Numerical) for various courses as detailed below:

1. **First two digits** indicate the code of college SJ
2. **Next three digits** indicate the programme/discipline code (ENG for English, MCM for M.Com, CHE for chemistry, PHY for physics, MLM for Malayalam, SKT for Sanskrit, HTY for History etc.)

3. **Sixth digit** is the Semester indicator which can be given as 1, 2, 3 & 4 respectively for I, II, III & IV Semester (MCM1, CHE2 etc.).
4. **Seventh digit** will be the Course Category indicator as detailed below :

Sl No	Nature of Course	Course Code
1	**C**ore Courses	**C**
2	**E**lective Courses	**E**
3	**P**roject	**P**
4	Comprehensive **V**iva	**V**
5	Practical / **L**ab	**L**
6	**A**udit Courses	**A**

5. **Last two digits** indicate the serial number of the respective courses. If there is one digit it should be prefixed by '0' (Zero). (01, 02, etc.)
6. If the number of courses in one category is only one (eg: Viva, Project etc.), assign the course serial number as 01.
7. Examples :

Sl. No	Code	Details
1	SJMCM1C01	M.Com I Sem Core Course No1
2	SJCHE2A02	Chemistry II Sem Audit Course No.2
3	SJENG4V01	English IV Sem Viva No. 1
4	SJMLM3E02	Malayalam III Sem Elective No. 2
5	SJPHY4P01	Physics IV Sem Project Work No. 1
6	SJBGY2L02	Biology II Sem Practical No. 2
7	SJPSY3C02	Psychology III Sem Core Coure No. 2
8	SJHTR2E01	History II Sem Elective Course No. 1

STRUCTURE OF THE PROGRAMME

Scheme- Core Course

The following table shows the structure of the programme which indicates course code, course title, instructional hours and credits.

Semester I						
Course Code	**Title of the course**	**Number of hours per week**	**Total Credits**	**Total hours/ semester**	**Marks**	
					SA	**ESA**
SJCHE1C01	Quantum Mechanics and Computational Chemistry	4	4	72	25	150
SJCHE1C02	Elementary inorganic chemistry	3	4	54	25	150
SJCHE1C03	Structure and reactivity of organic Compounds	3	4	54	25	150
SJCHE1C04	Thermodynamics, kinetics, and catalysis	3	4	54	25	150
Semester II						
SJCHE2C05	Group theory and Chemical Bonding	3	3	54	25	150
SJCHE2C06	Coordination chemistry	3	3	54	25	150
SJCHE2C07	Reaction mechanism in Organic Chemistry	3	3	54	25	150
SJCHE2C08	Electrochemistry, solid Thermodynamics	3	3	54	25	150
SJCHE2L04	Inorganic chemistry practical II	4	3	72	50	150
SJCHE2L05	Organic chemistry practical II	4	3	72	50	150
SJCHE2L06	Physical chemistry practical II	4	3	72	50	150
Semester III						
SJCHE3C09	Molecular spectroscopy	4	4	72	25	150
	Organometallic &					

SJCHE3C10	Bioinorganic chemistry	3	4	54	25	150
SJCHE3C11	Reagents and Transformations in Organic Chemistry	3	4	54	25	150
Semester IV						
SJCHE4C12	Instrumental Methods of Analysis	4	4	72	25	150
SJCHE4L10	Inorganic Chemistry Practical IV	3	3	54	25	150
SJCHE4L11	Organic Chemistry Practical IV	3	3	54	50	150
SJCHE4L12	Physical Chemistry Practical IV	3	3	54	50	150

Scheme- Elective Courses

Semester III						
Course Code	**Title of the course**	**Number of hours per week**	**Total Credits**	**Total hours/ semester**	**Marks**	
					SA	**ESA**
SJCHE3E01	Synthetic organic chemistry(Elective)	3	4	54	25	150
SJCHE3E02	Computational chemistry(Elective)	3	4	54	25	150
SJCHE3E03	Green and Nanochemistry(Elective)	3	4	54	25	150
Semester IV						
SJCHE4E04	Petrochemicals Cosmetics(Elective)	4	4	72	25	150
SJCHE4E05	Industrial Catalysis(Elective)	4	4	72	25	150
SJCHE4E06	Natural products & Polymer Chemistry (Elective)	4	4	72	25	150
SJCHE4E07	Material Science(Elective)	4	4	72	25	150
	Organometallic					

SJCHE4E08	Chemistry	4	4	72	25	150
SJCHE4E09	Medicinal & Combinatorial Chemistry	4	4	72	25	150

Scheme- Project work / dissertation and comprehensive viva-voce

Semester IV						
Course Code	**Title of the course**	**Number of hours per week**	**Total Credits**	**Total hours/ semester**	**Marks**	
					SA	**ESA**
SJCHE4P01	Research Project	3	4	54	50	150
SJCHE4V01	Viva Voce		2			

EVALUATION AND GRADING

The evaluation scheme for each course will contain two parts; (a) Internal/Continuous Assessment (CA) and (b) External / End Semester Evaluation (ESE). Of the total, 20% weightage will be given to internal evaluation/Continuous assessment and the remaining 80% to External/ESE and the ratio and weightage between Internal and External is 1:4.

a) Internal/Continuous Assessment (CA) : 20 marks

b) External / End Semester Evaluation (ESE) : 80 marks

Primary evaluation for Internal and External shall be based on 6 letter grades (A+, A, B, C, D and E) with numerical values (Grade Points) of 5, 4, 3, 2, 1 & 0 respectively. Grade

Point Average: Internal and External components are separately graded and the combined grade point with weightage 1 for Internal and 4 for external shall be applied to calculate the Grade Point Average (GPA) of each course. Letter grade shall be assigned to each course based on the categorization based on Ten-point Scale. There is no revaluation for PG programme (due to double valuation)

Evaluation of Audit Courses:

The examination and evaluation will be conducted by the college either in the normal structure or MCQ model from the Question Bank and other guidelines provided by the University/BoS. The Question paper will be for minimum 20 weightage and a minimum of 2-hour duration for the examination. The marks of audit courses one and two will be forwarded to Controller of Examinations of St. Joseph's College (Autonomous) Irinjalakuda in time of respective semesters. The result will be intimated / uploaded to the University during the Third Semester.

Phases for Evaluation:

I Phase: To be done by the concerned Teacher/Examiner based on 6 Point Scale

1. Evaluation of all individual External Theory courses and Internal evaluation

2. Evaluation of Project Work External and Internal

3. Evaluation of External and Internal Practical Courses

4. Evaluation of External and Internal Comprehensive Viva-voce

II Phase - GPA Calculation - To be done by St. Joseph's College (Autonomous)

1. Consolidation of External and Internal for Theory Courses (Calculation of GPA)

2. Consolidation of External and Internal for Project Work (Calculation of GPA)

3. Consolidation of External and Internal for Practical Courses (Calculation of GPA)

4. Consolidation of External and Internal for Comprehensive Viva-voce (Calculation of GPA)

III Phase - SGPA Calculation - To be done by St. Joseph's College (Autonomous) Irinjalakuda

- Calculation of Semester Grade Point Average. This is the consolidated net result (Grade) in a particular Semester.

IV Phase - CGPA Calculation - To be done by St. Joseph's College (Autonomous) Irinjalakuda

- Calculation of Consolidated Grade Point Average. This is the consolidated net result (Grade) of a programme.

Internal Evaluation / Continuous Assessment (CA)

Continuous Assessment will be based on a predetermined transparent system involving periodic two written tests, assignments, seminars and attendance in respect of theory courses and based on tests, lab skill and records/viva in respect of practical courses. The criteria and percentage of weightage assigned to various components for internal evaluation are as follows:

(a) Theory:			
Sl. No	**Component**	**Percentage**	**Weightage**
1	Examination /Test	40%	2

2	Seminars / Presentation	20%	1
3	Assignment	20%	1
4	Attendance	20%	1
(b) Practical:			
1	Lab Skill	40%	4
2	Records/viva	30%	3
3	Practical Test	30%	3

Attendance weightage 1 can be distributed as follows

Attendance	Internal weightage	Marks
Above 90%	1	5
85–89%	0.8	4
80–84%	0.6	3
76–79%	0.4	2
75%	0.2	1

Grades given for the internal evaluation are based on the grades A^+, A, B, C, D & E with grade points 5, 4, 3, 2, 1 & 0 respectively. The overall grades will be as per the Ten Point scale. There shall be no separate minimum Grade Point for internal evaluation. To ensure transparency of the evaluation process, the internal assessment marks awarded to the students in each course in a semester will be published on the notice board before 5 days of commencement of external examination. There will not be any chance for improvement of internal marks. The course teacher will maintain the academic record of each student registered for the course.

Examination /Test: For each course there shall be class test/s during a semester. Grades should be displayed on the notice board. Valued answer scripts shall be made available to the

students for perusal.

Seminars / Presentation: Every student should deliver Seminar/Presentation as an internal built –in component of the curriculum transaction for every course and must be evaluated by the respective course teacher in terms of structure, content, presentation and interaction. The soft and hard copies of the seminar report are to be submitted to the course teacher.

Assignment: Each student will be required to do assignment/s as an internal built – in component of the curriculum transaction for each course. Assignments after valuation must be returned to the students. The teacher shall define the expected quality of the above in terms of structure, content, presentation etc. and inform the same to the students. Punctuality in submission is to be considered.

Lab Skill: Students in the science stream are required to combine their classroom methods with hands on practical sessions in the laboratories. The teacher shall assess the skills of the student and the quality of application of theoretical knowledge.

Records/viva: Records are submitted by science students for documenting the textual and classroom knowledge along with their practical lab skills. Neatness, accuracy and precision are also evaluated here. Viva voce is conducted to assess the grasp of knowledge gained by the student and to test their communication skills in the translation of the knowledge.

Practical Test: It is conducted for students in the science stream to assess their scientific temper and application of theoretical knowledge. The sense of precision and accuracy is also taken into account.

External / End Semester Evaluation (ESE)

The semester-end examinations in theory courses will be conducted by the Controller of Examination St. Joseph's College (Autonomous), Irinjalakuda with question papers set by

external experts. The evaluation of the answer scripts will be done by examiners based on a well-defined scheme of valuation. The external evaluation will be done immediately after the internal valuation. The language of writing the examination should be English

Pattern of Questions for External/ESE:

Questions will be set to assess the knowledge acquired, standard, and application of knowledge, application of knowledge in new situations, critical evaluation of knowledge and the ability to synthesize knowledge. Due weightage will be given to each module based on content/teaching hours allotted to each module. The question will be prepared in such a way that the answers can be awarded A+, A, B, C, D, E Grades. Different types of questions shall be given different weightages to quantify their range given in the following model:

Sl. No.	Type of Questions	Individual weightage	Total Weightage	Number of questions to be answered
1	Short Answer type questions	2	2 x 4 = 8	4 out of 7
2	Short essay/ problem solving type	3	3 x 4 = 12	4 out of 7
3	Long Essay type questions	5	5 x 2 = 10	2 out of 4
Total			**30**	**18**

End Semester Evaluation in Practical Courses will be conducted and evaluated by both Internal and External Examiners. (*Write about Duration and pattern of practical external examinations*)

Component	Weightage

Physical & Theoretical Chemistry – theory courses	5
Physical Chemistry – practical courses	5
Inorganic Chemistry – theory courses	5
Inorganic Chemistry – practical courses	5
Organic Chemistry – theory courses	5
Organic Chemistry – practical courses	5
Total weightage	**30**

Evaluation of project work / dissertation

There will be External and Internal evaluation with the same criteria for Project Work done and the grading system shall be followed. One component among the Project Work evaluation criteria will be Viva-voce (Project Work related) and the respective weightage will be 40%. Consolidated Grade for Project Work is calculated by combining both the External and Internal in the Ratio of 4:1 (80% & 20%). For a pass in Project Work, a student has to secure a minimum of P Grade in External and Internal examination combined. If the students could not secure minimum P Grade in the Project work, they will be treated as failed in that attempt and the students may be allowed to rework and resubmit the same in accordance with the University exam stipulations. There shall be no improvement chance for Project Work. The External and Internal evaluation of the Project Work shall be done based on the following criteria and weightages as detailed below:

Sl. No	Criteria	% of weightage	Weightage External	Weightage Internal
1	Relevance of the topic and Statement of problem	20%	8	2

2	Methodology & Analysis	20%	8	2
3	Quality of Report & Presentation	20%	8	2
4	Viva-Voce	40%	16	4
Total Weightage		**100%**	**40**	**10**

Conduct of comprehensive viva-voce

There will be External and Internal Comprehensive Viva-voce; the External Conduct and internal Conduct of the Viva-voce are mandatory.

For a pass in Comprehensive viva-voce, a student has to secure a minimum of P Grade in External and Internal examination combined. If the students could not secure minimum P Grade in the Comprehensive viva-voce, they will be treated as failed in that attempt and the student may reappear for the same next time in accordance with the University exam stipulations. There shall be no improvement chance for Comprehensive viva-voce.

DIRECT GRADING SYSTEM

Direct Grading System based on a 10 – Point scale is used to evaluate the performance (External and Internal Examination of students). For all courses (Theory & Practical)/Semester/Overall Programme, Letter grades and GPA/**SGPA/CGPA** are given on the following way:

a) First Stage Evaluation for both Internal and External done by the Teachers concerned in the following Scale :

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

b) The Grade Range for both Internal & External shall be :

Letter Grade	Grade Range	Range of Percentage (%)	Merit / Indicator
O	4.25 – 5.00	85.00 –100.00	Outstanding
A+	3.75 – 4.24	75.00 – 84.99	Excellent
A	3.25 – 3.74	65.00 – 74.99	Very Good
B+	2.75 – 3.24	55.00 – 64.99	Good

B	2.50 – 2.74	50.00 – 54.99	Above Average
C	2.25 – 2.49	45.00 – 49.99	Average
P	2.00 -2.24	40.00 – 44.99	Pass
F	< 2.00	Below 40	Fail
I	0	-	Incomplete
Ab	0	-	Absent

'B 'Grade lower limit is 50% and 'B+' Grade lower limit is 55%

No separate minimum is required for internal evaluation for a pass, but a minimum P Grade is required for a pass in the external evaluation. However, a minimum P grade is required for pass in a course. A student who fails to secure a minimum grade for a pass in a course will be permitted to write the examination along with the next batch.

Improvement of Course - The candidates who wish to improve the grade / grade point of the external examination of a course/s they have passed already can do the same by appearing in the external examination of the concerned semester along with the immediate junior batch.

Betterment Programme One time - A candidate will be permitted to improve the CGPA of the Programme within a continuous period of four semesters immediately following the completion of the programme allowing only once for a particular semester. The CGPA for the betterment appearance will be computed based on the SGPA secured in the original or betterment appearance of each semester whichever is higher.

Semester Grade Point Average (SGPA) – Calculation

The SGPA is the ratio of sum of the product of the number of credits with the grade points scored by a student in all the courses taken by a student and the sum of the number of credits of all the courses taken by a student. After the successful completion of a semester, Semester Grade Point Average (SGPA) of a student in that semester is calculated using the formula given below.

Semester Grade Point Average - SGPA (S_j) = $\Sigma(C_i \times G_i) / Cr$
(SGPA= Total Credit Points awarded in a semester / Total credits of the semester)

Where 'S_j' is the j^{th} semester , 'G_i ' is the grade point scored by the student in the i^{th} course 'c_i ' is the credit of the i^{th} course,'Cr ' is the total credits of the semester .

Cumulative Grade Point Average (CGPA) – Calculation

Cumulative Grade Point Average (CGPA) = $\Sigma(C_i \times S_i) / Cr$(CGPA= Total Credit points awarded in all semesters/Total credits of the programme)

Where C_1 is the credit of the I^{st} semester S_1 is the SGPA of the I^{st} semester and Cr is the total number of credits in the programme. The CGPA is also calculated in the same manner taking into account all the courses undergone by a student over all the semesters of a programme. The SGPA and CGPA shall be rounded off to 2 decimal points. For the successful completion of a semester, a student should pass all courses and score a minimum SGPA of 2.0. However, the students are permitted to move to the next semester irrespective of their SGPA.

CONSOLIDATED SCHEME FOR I TO VI SEMESTERS

PROGRAMME STRUCTURE

SEMESTER I

COURSE CODE	COURSE TITLE	HOURS	CREDIT
SJCHE1C01	Quantum Mechanics and Computational Chemistry	72	4
SJCHE1C02	Elementary inorganic chemistry	54	4
SJCHE1C03	Structure and reactivity of organic Compounds	54	4
SJCHE1C04	Thermodynamics, kinetics, and catalysis	54	4

SEMESTER II

COURSE CODE	COURSE TITLE	HOURS	CREDIT
SJCHE2C05	Group theory and Chemical Bonding	54	3
SJCHE2C06	Coordination chemistry	54	3
SJCHE2C07	Reaction mechanism in Organic Chemistry	54	3
SJCHE2C08	Electrochemistry, solid Thermodynamics	54	3
SJCHE2L04	Inorganic chemistry practical II	72	3
SJCHE2L05	Organic chemistry practical II	72	3
	Physical chemistry		

SJCHE2L06	practical II	72	3

SEMESTER III

COURSE CODE	COURSE TITLE	HOURS	CREDIT
CHE3C09	Molecular spectroscopy	72	4
CHE3C10	Organometallic &Bioinorganic chemistry	54	4
CHE3C11	Reagents and Transformations in Organic Chemistry	54	4
CHE3E01	Synthetic organic chemistry(Elective)	54	4
CHE3E02	Computational chemistry(Elective)	54	4
CHE3E03	Green and Nanochemistry(Elective)	54	4

SEMESTER IV

COURSE CODE	COURSE TITLE	HOURS	CREDIT
SJCHE4C12	Instrumental Methods of Analysis	72	4
SJCHE4L10	Inorganic Chemistry Practical IV	54	3
SJCHE4L11	Organic Chemistry Practical IV	54	3
SJCHE4L12	Physical Chemistry Practical IV	54	3
	Petrochemicals		

SJCHE4E04	Cosmetics(Elective)	72	4
SJCHE4E05	Industrial Catalysis(Elective)	72	4
SJCHE4E06	Natural products & Polymer Chemistry (Elective)	72	4
SJCHE4E07	Material Science(Elective)	72	4
SJCHE4E08	Organometallic Chemistry	72	4
SJCHE4E09	Medicinal & Combinatorial Chemistry	72	4
SJCHE4P01	Research Project	54	4
SJCHE4V01	Viva Voce		2

M.Sc. CHEMISTRY - SEMESTER I

SJCHE1C01 - QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY
(4 Credits, 72 h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To analyze limitations of classical mechanics while applying to sub-atomic level.	To develop the ability for applying the principles of chemistry.	Z	F	5	-
CO2	To understand how quantum mechanics is applied, starting from simple systems to hydrogen / like atom/s.	To develop the ability for applying the principles of chemistry.	U	C	30	-
CO3	To understand the basic principles of computational chemistry.	To develop the ability for applying the principles of chemistry.	U	F	5	-
CO4	To apply the principles of computational chemistry to solve simple systems.	To develop the ability for applying the principles of chemistry.	A	P	10	-
CO5	To evaluate the validity of quantum mechanical treatment with experimental observations, in explaining sub atomic processes.	To develop the ability for applying the principles of chemistry.	E	C	5	-
CO6	To create a logical thinking habit in microscopic systems.	To develop the ability for applying the principles of chemistry.	C	C	5	-

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Introduction to Quantum Mechanics (9h)

Black body radiation and Planck's quantum postulate. Einstein's photoelectric equation, Schrodinger's wave mechanics, Detailed discussion of postulates of quantum mechanics – State function or wave function postulate, Born interpretation of the wave function, well behaved functions, orthonormality of wave functions; Operator postulate, operator algebra, linear and nonlinear operators, Non-commuting operators and the Heisenberg's Uncertainty principle, Laplacian operator, Hermitian operators and their properties, eigen functions and eigen values of an operator; Eigen value postulate, eigen value equation, Expectation value postulate; Postulate of time-dependent Schrödinger equation of motion, conservative systems and time- independent Schrödinger equation. Stationary states.

Unit 2: Quantum Mechanics of Translational & Vibrational Motions (9h)

Free particle in one-dimension; Particle in a one-dimensional box with infinite potential walls, important features of the problem; Particle in a one-dimensional box with one finite potential wall, Particle in a rectangular well, (no derivation), Significance of the problem, Introduction to tunneling; Particle in a three dimensional box, Separation of variables, degeneracy, Symmetry breaking.

One-dimensional harmonic oscillator (complete treatment):- Method of power series, Hermite equation and Hermite polynomials, recursion relation, wave functions, and energies, important features of the problem, harmonic oscillator model and molecular vibrations.

Unit: 3 Quantum Mechanics of Rotational Motion (9h)

Co-ordinate systems: - Cartesian, and spherical polar coordinates and their relationships. Planar rigid rotor (or particle on a ring), the Phi-equation, solution ofhe Phi-equation, One particle Rigid rotator (non-planar rigid rotator or particle on a sphere) (complete treatment): The wave equation in spherical polar coordinates, separation of variables, the Phi-equation and the Theta-equation and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials, Rodrigue's formula, spherical harmonics (imaginary and real forms), polar diagrams of spherical harmonics. Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta ((Lx, Ly, Lz), commutation relations between these operators, Ladder operator method for angular momentum, space quantization.

Unit 4: Quantum Mechanics of Hydrogen-like Atoms (9h)

Potential energy of hydrogen-like systems, the wave equation in spherical polar coordinates, separation of variables, the R, Theta and Phi equations and their solutions, Laguerre and associated Laguerre polynomials, wave functions and energies of hydrogen-like atoms, orbitals, radial functions and radial distribution functions and their plots, angular functions (spherical harmonics) and their plots. The postulate of spin by Uhlenbeck and Goudsmith, Dirac's relativistic equation for hydrogen

atom and discovery of spin (qualitative treatment), spin orbitals, construction of spin orbitals from orbitals and spin functions.

Unit 5: Approximation Methods in Quantum Mechanics (9h)

Many body problem and the need of approximation methods; Independent particle model; Variation method – variation theorem with proof, illustration of variation theorem using a trial function [e.g., x (a-x)] for particle in a 1D-box, variation treatment for the ground state of helium atom; Perturbation method – time- independent perturbation method (non-degenerate case only), illustration by application to particle in a ID-box with slanted bottom, perturbation treatment of the ground state of the helium atom.

Unit 6: Quantum Mechanics of Many-electron Atoms (9h)

Hartree's Self-Consistent Field method for atoms, Fock modification using spin orbitals & Hartree - Fock Self- Consistent Field (HF-SCF) method for atoms, the Fock operator; Pauli's antisymmetry principle - Slater determinants; Roothan's concept of basis functions: Slater type orbitals (STO) and Gaussian type orbitals (GTO).

Unit 7: Introduction to Computational Chemistry - I (9h)

Electronic structure of molecules – Basics of HF-SCF method of molecules (derivation not required). Classification of Computational Chemistry methods – Molecular mechanics methods (the concept of the force field) and Electronic structure methods, ab initio and semi-empirical methods, density functional theory (Basic idea only), Concept of electron correlation and post HF methods. (Elementary idea)

Unit 8: Introduction to Computational Chemistry – II (9h)

Basis set approximation in ab initio methods -classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization & diffuse basis sets, Pople-style basis sets, and their nomenclature. Simple calculations using Gaussian programme– The structure of a Gaussian input file, Types of keywords, Specification of molecular geometry using a) Cartesian coordinates and b) Internal coordinates. The Z-matrix, Z- matrices of some simple molecules like H_2, H_2O, formaldehyde ammonia and methanol.

References (for units 1 to 6)

1. F.L. Pilar, *Elementary Quantum Chemistry*, McGraw-Hill, 1968.
2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson EducationInc.,
3. P.W.AtkinsandR.S.Friedman,*Molecular Quantum Mechanics*, 4thEdition, Oxford

University Press,2005.

4. M.W. Hanna, *Quantum Mechanics in Chemistry*, 2nd Edition, W.A. Benjamin Inc., 1969.
5. Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983 (first Indian edition,Viva books,2003).
6. Thomas Engel, Quantum Chemistry & Spectroscopy, Pearson Education, 2006.
7. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc., 1993.
8. HoriaMetiu, *Physical Chemistry – Quantum Mechanics*, Taylor & Francis, 2006.
9. A.K. Chandra, *Introduction to Quantum Chemistry*, 4th Edition, Tata McGraw- Hill, 1994.
10. L. Pauling and E.B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1935 (A good source book for many derivations).
11. R.L. Flurry, Jr., *Quantum Chemistry*, Prentice Hall, 1983.
12. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006.
13. M.S. Pathania, *Quantum Chemistry, and Spectroscopy (Problems & Solutions)*, Vishal Publications, 1984.
14. C.N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry*, Prism Books Pvt. Ltd. 1998.
15. Jack Simons, *An Introduction to Theoretical Chemistry*, Cambridge University Press, 2003.

References (for units 7 & 8)

1. C. J. Cramer, *Essentials of computational Chemistry: Theories and models*, John Wiley & Sons 2002.
2. Frank Jensen, *Introduction to Computational Chemistry*, John Wiley & Sons LTD1999.
3. J. Foresman &Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.
4. David Young, *Computational Chemistry- A Practical Guide for Applying Techniques to Real- World Problems"*, Wiley -Interscience, 2001.
5. Errol G. Lewars, *Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics*, 2 nd edn., Springer2011.

M.Sc. CHEMISTRY - SEMESTER I

SJCHE1C02 - ELEMENTARY INORGANIC CHEMISTRY
(4 Credits, 54 h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the basic principles of bonding	To develop the ability for applying the principles of chemistry.	A	F	10	-
CO2	To understand the periodic table	To develop the ability for applying the principles of chemistry.	A	C	5	-
CO3	To understand the chemistry of Elements.	To develop the ability for applying the principles of chemistry.	A	C	10	-
CO4	To understand the nuclear chemistry.	To develop the ability for applying the principles of chemistry.	U	F	10	-
CO5	To understand the concepts of acids and bases.	To develop the ability for applying the principles of chemistry.	C	C	10	-
CO6	To study about nanomaterials.	To develop the ability for applying the principles of chemistry.	E	C	5	-

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Concepts of Acids and Bases (9h)

Major acid-base concepts, Arrhenius, Bronsted-Lowry, Solvent system, Lux-Flood, Lewis and Usanovich concepts. Classification of acids and bases as hard and soft. HSAB principle. The theoretical basis of hardness and softness. The Drago-Wayland equation, E and C parameters-Symbiosis. Applications of HSAB concept. Chemistry of nonaqueous solvents- NH_3, SO_2, H_2SO_4, BrF_3, HF, N_2O_4, and HSO_3F. Nonaqueous solvents and acid-base strength. Super acids–surface acidity.

Unit 2: Chemistry of Main Group Elements-I (9h)

Chemical periodicity-First and Second raw anomalies-The diagonal relationship- Periodic anomalies of the nonmetals and post-transition metals. Allotropes of C, S, P. As, Sb, Bi, O, and Se. Electron-deficient compounds-Boron hydrides-preparation, reactions, structure, and bonding. Styx numbers-closo, nido, arachno polyhedral structures. Boron cluster compounds-Wade's rule. Polyhedral borane anion-carboranes, metallaboranes and metallacarboranes. Borazines and borides.

Unit 3: Chemistry of Main Group Elements-II (9h)

Silicates and alumino silicates-Structure, molecular sieves-Zeolite. Silicones- Synthesis, structure and uses. Carbides and silicides. Synthesis, structure, bonding, and uses of Phosphorous-Nitrogen, Phosphorous-Sulphur, and Sulphur-Nitrogen compounds.

Unit 4: Chemistry of Transition and Inner Transition Elements (9h)

Heteropoly and isopoly anions of W, Mo, V.Standard reduction potentials and their diagrammatic representations Ellingham diagram. Latimer and Frost diagrams. Pourbaix diagram.Differences between 4f and 5f orbitals. Magnetic and spectroscopic properties. Uranyl compounds. Trans-actinide elements. Super heavy elements : production and chemistry.

Unit 5: Nuclear and Radiation Chemistry (9h)

Structure of nucleus: shell, liquid drop, Fermi gas, collective and optical models. Nuclear reaction: Bethe`s notation of nuclear process- Types-reaction cross section- photonuclear and thermonuclear reactions. Nuclear fission: Theory of fission- neutron capture cross section and critical size. Nuclear fusion. Neutron activation analysis. Radiation chemistry: Interaction of radiation with matter. Detection and measurement of radiation- GM and scintillation counters – radiolysis of water- radiation hazards- radiation dosimetry.

Unit 6: Chemistry of Nanomaterials (9h)

History of nanomaterials-Classification. Size - dependence of properties. Synthesis of nanostructures: bottom-up-approach, top-down approach, self-assembly lithography, molecular synthesis, template-assisted synthesis. Methods of characterization: Electron microscopies-SEM, TEM. Scanning probe microscopies- STM, AFM. X-ray photoelectron spectroscopy (XPS),

Dynamic light scattering (DLS), and X-ray diffraction (XRD) .Applications: Nanoelectronics, nanosensors, nanocatalysts, nanofiltration, diagnostic and therapeutic applications, and targeted drug delivery. Introduction to graphenes and fullerenes.

References (for units 1 to 5)

1. N.N. Greenwood and A.Earnshaw, *Chemistry of Elements, 2/e, Elsevier* Butterworth- Heinemann, 2005.
2. J.E.Huheey, E.A.Keiter, R.L.Keiter. O.K.Medhi. *Inorganic Chemistry, principles of structure and reactivity*, Pearson Education, 2006.
3. G.L.Miessler, D.A.Tarr, *Inorganic Chemistry*, Pearson, 2010.
4. D.F.Shriver, P.W.Atkins, *Inorganic Chemistry*, Oxford University Press, 2002 5.William W Porterfield, *Inorganic Chemistry-Aunified approach*, AcademicPress, 2005.
5. Keith F Purcell, John C Kotz, *Inorganic Chemistry*, Cengage Learning, 2010.
6. James E House, *Inorganic Chemistry*, Academic Press, 2008.
7. H.J.Arnikar, *Essentials of Nuclear chemistry*, New Age International, 2005.
8. Friedlander and J.W.Kennedy, *Introduction to Radiochemistry*, John Wiley and Sons, 1981.
9. S. Glastone, *Source Book on Atomic Energy*, *3rd*edn., Affiliated East-West Press Pvt.Ltd., 1967.

References (for unit 6):

1. C.P.Poole(Jr.) and F.J. Owens, *Introduction to Nanotechnology*,Wiley India,2007.
2. G.A.Ozin and A.C.Arsenault, *Nanochemistry*, RSCPublishing, 2008.
3. T.Pradeep, *The essentials of Nanotechnology*, Tata McGraw-Hill, New Delhi, 2007.
4. K.J.Klabunde(Ed.), *Nanoscale Materials in Chemistry*, John Wiley&Sons,2001.

M.Sc. CHEMISTRY - SEMESTER I

SJCHE1C03 - STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS
(4 Credits, 54 h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To identify the bonding in organic molecules	To develop the ability for applying the principles of chemistry.	Z	F	10	-
CO2	To identify the structure of organic molecules	To develop the ability for applying the principles of chemistry.	A	C	5	-
CO3	To predict the reactivity of organic molecules	To develop the ability for applying the principles of chemistry.	A	C	10	-
CO4	To understand the stereochemistry of the compounds.	To develop the ability for applying the principles of chemistry.	U	F	9	-
CO5	To predict the synthetic routes for asymmetric compounds	To develop the ability for applying the principles of chemistry.	C	C	10	-
CO6	To study about the conformations of molecules	To develop the ability for applying the principles of chemistry.	E	C	8	-

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Structure and Bonding in Organic Molecules (9h)

Nature of Bonding in Organic Molecules: Localized and delocalized chemical bonding, bonding weaker than the covalent bond, cross- conjugation, resonance, rules of resonance, resonance hybrid and resonance energy, tautomerism, hyperconjugation, π-π interactions, pπ-dπ bonding (ylides).

Hydrogen bonding: Inter and intra-molecular hydrogen bonding. Range of the energy of hydrogen bonding. Effect of hydrogen bond on conformation, physical and chemical properties of organic compounds- volatility, acidity, basicity, and stability. Stabilization of hydrates of glyoxal and chloral, and ninhydrin. High acid strength of maleic acid compared to fumaric acid. Electron donor-acceptor complexes, crown ether complexes, cryptates, inclusion compounds, and cyclodextrins.

Hückel MO method. MO's of simple molecules, ethylene, allyl radical and 1, 3- butadiene. Hückel rule and modern theory of aromaticity, criteria for aromaticity and antiaromaticity, MO description of aromaticity and antiaromaticity.

Homoaromaticity. Aromaticity of annulenes and hetero annulenes, fused ring systems, fulvenes, fulvalenes, azulenes, pentalenes, and heptalenes. Preparation of aromatic and antiaromatic compounds by different methods, the stability of benzylic cations and radicals. Effect of delocalized electrons on pKa.

Unit 2: Structure and Reactivity (9h)

Transition state theory, Potential energy vs reaction co-ordinate curve, substituent effects (inductive, mesomeric, inductomeric, electromeric and field effects) on reactivity. A qualitative study of substitution effects in SN1- SN2 reactions. Neighbouring group participation, the participation of carboxylate ion, halogen, hydroxyl group, acetoxy group, phenyl group and pi -bond. Classical and nonclassical carbocations

Basic concepts in the study of organic reaction mechanisms: Application of experimental criteria to mechanistic studies, kinetic versus thermodynamic control- Hammond postulate, Bell- Evans- Polanyi principle, Marcus equation, Curtin- Hammet principles, Acidity constant, Hammet acidity function.

Isotope effect (labeling experiments), stereochemical correlations. Semiquantitative study of substituent effects on the acidity of carboxylic acids. Quantitative correlation of substituent effects on reactivity. Linear free energy relationships. Hammet and Taft equation for polar effects and Taft's steric substituent constant for steric effect. Solvent effects.

Unit 3: Conformational Analysis – I (9h)

Factors affecting the conformational stability of molecules – dipole interaction, bond opposition strain, bond angle strain. Confirmation of acyclic compounds – Ethane, n-butane, alkene dihalides, glycols, chlorohydrins, tartaric acid, erythro and threoisomer.

Interconversion of axial and equatorial bonds in chair conformation of cylohexane– distance between the various H atoms and C atoms in chair and boat conformations. Monosubstituted cyclohexane–methyl and t-butyl cyclohexanes–flexible and rigid systems. Confirmation of substituted cyclohexanone, 2-bromocyclohexanone, dibromocyclohexanone, (cis & trans), 2-bromo-4, 4-dimethyl cyclohexanone. Anchoring group and conformationaly biased molecules. Conformations of 1, 4 -cis and-trans disubstituted cyclohexanes in which one of the substituents is 1-butyl and their importance in assessing the reactivity of an axial or equatorial substituent.

Unit 4: Conformational Analysis – II (9 h)

Effect of conformation on the course and rate of reactions in (a) debromination of dl and meso 2, 3-dibromobutane or stilbene dibromide using KI. (b) semipinacolic deamination of erythro and threo 1,2-diphenyl-1-(p-chlorophenyl)-2-aminoethanol.

(c) dehydrohalogenation of stilbene dihalide (dl and meso) and erythro and threo- bromo-1,2-diphenyl propane.

Effect of conformation on the course and rate of reactions in cyclohexane systems illustrated by (a) SN2 and SN1 reactions for (i) an axial substituent, and (ii) an equatorial substituent inflexible and rigid systems. (b) E1, E2 eliminations illustrated by the following compounds. (i) 4-t-Butylcyclohexyl tosylate (cis and trans) (ii) 2- Phenylcyclohexanol (cis and trans) (iii) Menthyl and neomenthyl chlorides and benzene hexachlorides. (c) Pyrolytic elimination of esters (cis elimination) (d) Esterification of axial as well as equatorial hydroxyl and hydrolysis of their esters in rigid and flexible systems. (Compare the rate of esterification of methanol, isomenthol, neomenthol, and neoisomenthol). (f) Esterification of axial as well as equatorial carboxyl groups and hydrolysis of their esters. (g) Hydrolysis of axial and equatorial tosylates. (h) Oxidation of axial and equatorial hydroxyl group to ketones by chromic acid.

Bredt's rule. Stereochemistry of fused, bridged and caged ring systems- decalins, norbornane, barrelene, and adamantanes.

Unit 5: Stereochemistry (9h)

Conformation and configuration, Fischer, Newman, and Sawhorse projection formulae and their interconversion. Concept of chirality, recognition of symmetry elements and chiral structures, conditions for optical activity, optical purity. Specific rotation and its variation in sign and magnitude under different conditions, relative and absolute configurations, Fisher projection formula, sequence rule – R and S notation in cyclic and acyclic compounds, Cahn-Ingold- Prelog (CIP) rule. Mixtures of stereoisomers; enantiomeric excess and diastereomeric excess and their determination. Methods of resolution diastereomers. Resolution of racemates after conversion into diastereomers; use of S- brucine, kinetic resolution of enantiomers, chiral chromatography.

Optical isomerism of compounds containing one or more asymmetric carbon atoms, enantiotopic, homotopic, diastereotopic hydrogen atoms, prochiral centre. Pro-R, Pro-S,Re, and Si.

Optical isomerism in biphenyls, allenes, and nitrogen and sulphur compounds, conditions for optical activity, R and S notations. Optical activity in cis-trans conformational isomers of 1, 2-, 1, 3- and 1,4-dimethylcyclohexanes.Restricted rotation in biphenyls – Molecular overcrowding. Chirality due to the folding of helicalstructures.

Geometrical isomerism – E and Z notation of compounds with one and more double bonds in acyclic systems. Configuration of cyclic compounds- monocyclic, fused and bridged ring systems, interconversion of geometrical isomers. Methods of determination of the configuration of geometrical isomers in acyclic acid cyclic systems, the stereochemistry of aldoximes and ketoximes

Unit 6: Asymmetric Synthesis (9 h)

Asymmetric synthesis, need for asymmetric synthesis, stereoselectivity and stereospecificity. Chiral pool: chiral pool synthesis of beetle pheromone component (S)- (–)-ipsenol from (S)-(–)-leucine.

Classification of Asymmetric reactions into (1) Substrate controlled (2) Chiral auxiliary controlled (3) Chiral reagent controlled and (4) Chiral catalyst controlled.

1. Substrate controlled asymmetric synthesis: Nucleophillic addition to chiral carbonyl compounds. 1,2-asymmetric induction, Cram's rule and Felkin-Anh model.

2. Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, azaenolates, imines and hydrazones, chiral sulfoxides. 1,4-Asymmetric induction and Prelog's rule. Use of chiral auxiliary in Diels-Alder and Cope reactions.

3. Chiral reagent controlled asymmetric synthesis: Asymmetric reduction using BINAL – H. Asymmetric hydroboration using IPC2BH and IPCBH2. Reduction with CBS reagent. Stereochemistry of Sharpless asymmetric epoxidation and dihydroxylation

4. Asymmetric aldol reaction: Diastereoselective aldol reaction and its explanation by Zimmermann-Traxler model.

Chiral catalyst: Rhodium and Ruthenium catalysts with chiral phospine ligands like (R)BINAP, (S) BINAP, (R,R)DIOP

References:

1. R. R. Carey and R. J. Sundburg, Advanced Organic Chemistry, Part A, Springer, 5/e, 2007.

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6. M. S. Singh, Advanced Organic Chemistry: Reactions and Mechanisms, Pearson, 2013.
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10. G. L. D. Krupadanam, Fundamentals of Asymmetric Synthesis, Universities Press, 2013.
11. Okuyama and Maskill, Organic Chemistry: A Mechanistic Approach, Oxford University Press,2013
12. S. Warren and P. Wyatt, Organic Synthesis: The Disconnection Approach, 2/e, John Wiley & Sons, 2008.

M.Sc. CHEMISTRY - SEMESTER I

SJCHE1C04 - THERMODYNAMICS, KINETICS, AND CATALYSIS
(4 Credits, 54 h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To remember the basic principles of classical thermodynamics.	To develop the ability for applying the principles of chemistry.	R	F	5	-
CO2	To understand the need for irreversible thermodynamics.	To develop the ability for applying the principles of chemistry.	U	F	5	-
CO3	To apply the principles of irreversible thermodynamics in different irreversible processes.	To develop the ability for applying the principles of chemistry.	A	C	15	-
CO4	To analyze the kinetics of complex chemical reactions.	To develop the ability for applying the principles of chemistry.	Z	C	10	-
CO5	To understand the higher level chemistry of molecular dynamics	To develop the ability for applying the principles of chemistry.	U	C	10	-
CO6	To understand and to apply various analysis techniques in studying surface chemistry and catalysis.	To develop the ability for applying the principles of chemistry.	U	F	15	-

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Thermodynamics (9h)

Review of First and Second law of thermodynamics, Third law of thermodynamics, Need for third law, Nernst heat theorem, Apparent exceptions to third law, Applications of Third law, Determination of Absolute entropies, Residual entropy. Thermodynamics of Solutions: Partial molar quantities, Chemical potential, Variation of chemical potential with temperature and pressure, Partial molar volume and its determination, Gibbs-Duhem equation, Thermodynamics of ideal and real gases and gaseous mixtures, Fugacities of gases and their determinations, Activity, Activity coefficient, standard state of substance (for solute and solvents), Duhem- Margules equation and its applications. Thermodynamics of ideal solutions, Deduction of the laws of Raoult's ebullioscopy, cryoscopy, and osmotic pressure. Non-ideal solutions, Deviations from Raoult's law, Excess functions- excess free energy, excess entropy, excess enthalpy, excess volume.

Unit 2: Thermodynamics of Irreversible Processes (9 h)

Simple examples of irreversible processes, general theory of non-equilibrium processes, entropy production, the phenomenological relations, Onsager reciprocal relations, application to the theory of diffusion, thermal diffusion, thermo-osmosis, and thermo- molecular pressure difference, electro-kinetic effects, the Glansdorf- Pregogine equation.

Unit 3: Chemical Kinetics (9 h)

Kinetics of reactions involving reactive atoms and free radicals - Rice - Herzfeld mechanism and steady state approximation in the kinetics of organic gas phase decompositions (acetaldehyde & ethane); Kinetics of chain reactions – branching chain and explosion limits (H_2-O_2reaction as an example); Kinetics of fast reactions- relaxation methods, molecular beams, flash photolysis; Solution kinetics: Factors affecting reaction rates in solution, Effect of solvent and ionic strength (primary salt effect) on the rate constant, secondary salt effects.

Unit 4: Molecular Reaction Dynamics (9 h)

Reactive encounters: Collision theory, diffusion-controlled reactions, the material balance equation, Activated Complex theory – the Eyring equation, thermodynamic aspects of ACT; Comparison of collision and activated complex theories; The dynamics of molecular collisions – Molecular beams, principle of crossed-molecular beams; Potential energy surfaces - attractive and repulsive surfaces, London equation, Statistical distribution of molecular energies; Theories of unimolecular reactions - Lindemann's theory, Hinshelwood's modification, Rice -Ramsperger and Kassel (RRK) model.

Unit 5: Surface Chemistry (9 h)

Structure and chemical nature of surfaces, Adsorption at surfaces - Adsorption isotherms, Langmuir's unimolecular theory of adsorption, BET equation, derivation, Determination of surface area and pore structure of adsorbents - physical adsorption methods, X-ray methods, mercury intrusion method, chemisorption methods. Determination of surface acidity-TPD method. Heat of adsorption and its determination.

Unit 6: Catalysis (9h)

Features of homogeneous catalysis–Enzyme catalysis - Michaelis-Menten Mechanism.Features of heterogeneous catalysis -Langmuir-Hinshelwood mechanism and Eley-Rideal mechanism – illustration using the reaction $2CO + O_2 \dashrightarrow 2CO_2$. Methods of preparation of heterogeneous catalysts - precipitation and co- precipitation methods, sol gel method, flame hydrolysis. Preparation of Zeolites and silica supports. Auto catalysis - oscillating reactions – mechanisms of oscillating reactions (Lotko -Volterra, brusselator, and oregonator). Introduction to Phase transfer catalysis, biocatalysis, nanocatalysis, and polymer supported catalysis.

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15. Jens Hajen, *Industrial Catalysis: A Practical Approach.* 2nd Edn, Wiley VCH, 2006.
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M.Sc. CHEMISTRY - SEMESTER II

SJCHE2C05 - GROUP THEORY AND CHEMICAL BONDING
(4 Credits, 54 h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the basic principles of group theory	To develop the ability for applying the principles of chemistry.	R	F	4	-
CO2	To study some theorems in Group theory	To develop the ability for applying the principles of chemistry.	U	C	10	-
CO3	To understand how group theory is applied in molecular spectroscopy	To develop the ability for applying the principles of chemistry.	z	F	10	-
CO4	To understand how group theory is applied in in chemical bonding	To develop the ability for applying the principles of chemistry.	A	P	10	-
CO5	To validate VBT and MOT in diatomic molecules	To develop the ability for applying the principles of chemistry.	E	C	10	-
CO6	To analyze the feasibility of MOT in polyatomic molecules.	To develop the ability for applying the principles of chemistry.	A	c	8	-

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Foundations of Group Theory & Molecular Symmetry (9h)

Basic principles of group theory - the defining properties of mathematical groups, finite and infinite groups, Abelian and cyclic groups, group multiplication tables (GMT), similarity transformation, sub groups & classes in a group. Molecular Symmetry & point groups - symmetry elements and symmetry operations in molecules, relations between symmetry operations, complete set of symmetry operations of a molecule, point groups and their systematic identification, GMT of point groups. Mathematical preliminaries - matrix algebra, addition and multiplication of matrices, inverse of a matrix, square matrix, character of a square matrix, diagonal matrix, direct product and direct sum of square matrices, block factored matrices, solving linear equations by the method of matrices; Matrix representation of symmetry operations.

UNIT 2: Representations of Point Groups& Corresponding Theorems (9h)

Representations of point groups - basis for a representation, representations using vectors, atomic orbitals and Cartesian coordinates positioned on the atoms of molecule (H_2O as example) as bases, reducible representations and irreducible representations (IR) of point groups, construction of IR by reduction (qualitative demonstration only), Great Orthogonality Theorem (GOT) (no derivation) and its consequences, derivation of characters of IR using GOT, construction of character tables of point groups (C_{2V}, C_{3V}, C_{2h} and C_{4V} and C_3 as examples), nomenclature of IR- Mulliken symbols, symmetry species. Reduction formula - derivation of reduction formula using GOT, reduction of reducible representations, (e.g.,Γ_{cart}) using the reduction formula. Relation between group theory and quantum mechanics – wavefunctions (orbitals) as bases for IR of point groups.

Unit 3: Applications of Group Theory to Molecular Spectroscopy (9h)

Molecular vibrations - symmetry species of normal modes of vibration, construction of Γ_{cart}, normal coordinates and drawings of normal modes (e.g., H_2O and NH_3), selection rules for IR and Raman activities based on symmetry arguments, determination of IR active and Raman active modes of molecules (e.g., H_2O, NH_3, CH_4 , SF_6), complementary character of IR and Raman spectra. Spectral transition probabilities - direct product of irreducible representations and its use in identifying vanishing and non–vanishing integrals, transition moment integral and spectral transition probabilities. Electronic Spectra – electronic transitions and selection rules, Laporte selection rule for centro symmetric molecules.

Unit 4: Applications of Group Theory to Chemical Bonding (9h)

Hybridization - Treatment of hybridization in BF_3 and CH_4, Inverse transformation and construction of hybrid orbitals. Molecular orbital theory – HCHO and H_2O as examples, classification of atomic orbitals involved into symmetry species, group orbitals, symmetry adapted linear combinations (SALC), projection operator, construction of SALC using projection operator, use of projection operator in constructing SALCs for the Π MOs in cyclopropenyl ($C_3H_3^+$)cation.

Unit 5: Chemical bonding in diatomic molecule (9h)

Schrödinger equation for a molecule, Born – Oppenheimer approximation; Valence Bond (VB) theory – VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2; Molecular Orbital (MO) theory – MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules – Li_2, Be_2, C_2, N_2, O_2 & F_2 and heteronuclear diatomic molecules – LiH, CO, NO & HF, bond order, correlation diagrams, non-crossing rule; Spectroscopic term symbols for diatomic molecules; Comparison of MO and VB theories.

Unit 6: Chemical Bonding in polyatomic molecules (9h)

Hybridization – quantum mechanical treatment of sp, sp^2 & sp^3 hybridisation. Semi empirical MO treatment of planar conjugated molecules – Hückel Molecular Orbital (HMO) theory of ethylene, butadiene & allylic anion. Charge distribution, and bond orders from the coefficients of HMO, calculation of free valence. HMO theory of aromatic hydrocarbons (benzene); formula for the roots of the Hückel determinantal equation, Frost -Hückel circle mnemonic device for cyclic polyenes.

Reference (for Units 1 to 4)

1. F.A. Cotton, *Chemical applications of Group Theory*, 3rdEdition, John Wiley &Sons Inc.,2003.
2. H. H. Jaffe and M. Orchin, *Symmetry in Chemistry*, John Wiley &Sons Inc., 1965.
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Reference (for units 5 &6)

1. F.L. Pilar, *Elementary Quantum Chemistry*, McGraw-Hill, 1968.
2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson EducationInc.,
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6. Thomas Engel, *Quantum Chemistry & Spectroscopy*, Pearson Education, 2006.
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8. A.K. Chandra, *Introduction to Quantum Chemistry*, 4th Edition, Tata McGraw-Hill, 1994.
9. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006.
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M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER II

SJCHE2C06 - CO-ORDINATION CHEMISTRY (3Credits, 54 h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the basic concept in coordination chemistry	To develop the ability for applying the principles of chemistry.	U	F	7	-
CO2	To study the feasibility of MOT and CFT in coordination compounds	To develop the ability for applying the principles of chemistry.	Z	C	10	-
CO3	To study the mechanism of substitution reactions	To develop the ability for applying the principles of chemistry.	A	F	7	-
CO4	To evaluate the magnetic properties of complexes.	To develop the ability for applying the principles of chemistry.	R	C	9	-
CO5	To understand the photochemical reactions of complexes	To develop the ability for applying the principles of chemistry.	E	C	10	-
CO6	To analyze the Characterizations techniques in coordination chemistry	To be exposed to the different processes used in industries and their applications	Z	F	9	-

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Stability of Co-ordination Compounds (9h)

Stereochemistry of coordination compounds. Stepwise and overall formation constants and the relationship between them. Trends in stepwise formation constants. Determination of binary formation constants by pH-metry and spectrophotometry. Stabilization of unusual oxidation states. Ambidentate and macrocyclic ligands. Chelate effect and its thermodynamic origin. Macrocyclic and template effects.

Unit 2: Theories of Bonding in Coordination Compounds (9h)

Sidgwick`s electronic interpretation of coordination. The valence bond theory and its limitations. The crystal field and ligand field theories. Splitting of d-orbitals in octahedral, tetrahedral and square planar fields. Factors affecting crystal field splitting. Spectrochemical and nephelauxetic series. Racah parameters. Jahn-Teller effect. Molecular orbital theory-composition of ligand group orbitals. MO diagram of octahedral, tetrahedral and square planar complexes. Π-bonding and molecular orbital theory.

Unit 3: Electronic Spectra and Magnetic Properties of Complexes (9h)
Spectroscopic ground state. Terms of d^n configurations. Selection rules for d-d transitions. Effect of ligand fields on RS terms in octahedral and tetrahedral complexes. Orgel diagrams. Calculation of D_q, B, and β parameters. Tanabe-Sugano diagrams. Charge transfer spectra.

Types of magnetic properties: Paramagnetism and diamagnetism. Curie and Curie-Weiss laws.Theμ_J, μ_{L+S}, and μ_S expressions. Orbital contribution to magnetic moment and its quenching. Spin-orbit coupling. Temperature independent paramagnetism. Antiferromagnetism- types and exchange pathways. Determination of magnetic moment by Gouy method.

Unit 4: Characterization of Coordination Complexes (9h)

Infrared spectra of metal complexes. Group frequency concept. Changes in ligand vibrations on coordination- metal ligand vibrations. Application in coordination complexes. ESR spectra – application to copper complexes. NMR spectroscopy for structural studies of diamagnetic metal complexes from chemical shift and spin- spin coupling. Mossbauer spectroscopy- the Mossbauer Effect, hyperfine interactions (qualitative treatment). Application to iron and tin compounds.

Unit 5: Reaction Mechanism of Metal Complexes (9h)

Ligand substitution reactions. Labile and inert complexes. Rate laws. Classification of mechanisms-D, A and I mechanisms. Substitution reactions in octahedral complexes. The Eigen-Wilkins Mechanism. Fuoss-Eigen equation. Aquation and base hydrolysis-mechanism.

Substitution reactions in square planar complexes. The trans effect: Applications and theories of trans effect. The cis effect.

Unit 6: Redox and Photochemical Reactions of Complexes (9h)

Classification of redox reaction mechanisms. Outer sphere and inner sphere mechanisms. Marcus equation. Effect of the bridging ligand. Methods for distinguishing outer- and inner-sphere redox reactions.

Photochemical reactions of metal complexes: Prompt and delayed reactions. Excited states of metal complexes- Interligand, ligand field, charge transfer, and delocalized states. Properties of ligand field excited states. Photosubstitution- Prediction of substitution lability by Adamson`s rules. Photoaquation. Photo isomerization and photo racemization. Illustration of reducing and oxidizing character of $[Ru(bipy)_3]^{2+}$ in the excited state. Metal complex sensitizers- water photolysis.

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M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER II

SJCHE2C07 - REACTION MECHANISM IN ORGANIC CHEMISTRY

(3 Credits, 54h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand common substitution and elimination reactions.	To develop the ability for applying the principles of chemistry.	U	F	9	-
CO2	To interpret structure and synthesis of various natural products.	To develop the ability for applying the principles of chemistry.	U	C	9	-
CO3	To analyse the role of intermediates in common reactions.	To be exposed to the different processes used in industries and their applications	Z	C	3	-
CO4	To analyse the mechanistic aspects of various name reactions.	To develop the ability for applying the principles of chemistry.	Z	C	7	-
CO5	To apply the principles of pericyclic reactions.	To develop the ability for applying the principles of chemistry.	A	C	9	-
CO6	To apply the photochemical reactions in various organic molecules.	To develop the ability for applying the principles of chemistry	A	C	9	-

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Aliphatic and Aromatic Substitutions (9 h)

Nucleophilic Aliphatic Substitution: Mechanism and Stereochemistry of S_N2 and S_N1 reactions. Ion-pair mechanism. The effect of substrate structure, reaction medium, nature of leaving group and nucleophile on S_N2 and S_N1 reactions. S_Ni and neighboring group mechanism. SET mechanism. Allylic and benzylic substitutions. Ambident nucleophiles and substrates regioselectivity.

Electrophilic Aliphatic Substitution: Mechanism and stereochemistry of S_E1, S_E2 (front), S_E2 (back) and S_Ei reactions. The effect of substrate structure, leaving group and reaction medium on S_E1 and S_E2 reactions.

Electrophilic Aromatic Substitution: Arenium ion mechanism, substituent effect on reactivity in mono and disubstituted benzene rings, *ortho/para* ratio, *Ipso* substitution. Relationship between reactivity and selectivity. Nucleophilic Aromatic substitution: Addition- elimination (S_NAr) mechanism, elimination-addition (benzyne) mechanism, *cine* substitution, S_N1 and $S_{RN}1$ mechanism. The effect of substrate structure, nucleophile and leaving group on aromatic nucleophilic substitution.

Unit 2: Addition & Elimination Reactions and Reactive Intermediates (9h)

(i) Addition and Elimination Reactions (6h)

Mechanistic and stereochemical aspects of addition to C=C involving electrophiles, nucleophiles and free radicals. Effect of substituents on the rate of addition, orientation of addition, addition to conjugated systems and cyclopropane rings, Michael reaction.

Mechanistic and stereochemical aspects of E1, E1cB and E2 eliminations. The effect of substrate structure, base, leaving group and reaction medium on elimination reactions. Saytzev *vs* Hofmann elimination, α- elimination, pyrolytic *syn* elimination (E*i*) and conjugate eliminations. Competition between substitution and elimination reactions, basicity *vs* nucleophilicity. Extrusion reactions- extrusion of N_2, CO and CO_2.

(ii)Reactive Intermediates (3hrs)

Reactive Intermediates: Generation, geometry, stability, and reactions of carbonium ions and carbanions, free radicals, carbenes, nitrenes and benzynes.

Unit 3: Chemistry of Carbonyl Compounds (9h)

(i)Reactions of Carbon-heteromultiple Bonds (7h)

Reactivity of carbonyl compounds toward addition, mechanistic aspects of hydration addition of alcohols, and condensation with nitrogen nucleophiles to aldehydes and ketones. Addition of organometallic reagents- Grignard reagents- organozinc, organocopper and organolithium reagents- to carbonyl compounds. Aldol, Perkin, Claison, Dieckmann, Stobbe, and benzoin condensation. Darzen's, Knoevenagel, Reformatsky, Wittig, Cannizaro, Mannich, and Prins reactions. MPV reduction and Oppenauer oxidation.

Addition to carbon-nitrogen multiple bonds: Ritter reaction and Thorpe condensation. Hydrolysis, alcoholysis, and reduction of nitriles.

(ii)Esterification and Ester Hydrolysis (2h): Mechanisms of ester hydrolysis and esterification, Acyl-oxygen and alkyl oxygen cleavage.

Unit 4: Pericyclic Reactions (9 h)

Phase and symmetry of molecular orbitals, FMOs of ethylene, 1, 3- butadiene, 1, 3, 5-hexatriene, allyl, and 1, 3-pentadienyl systems. Pericyclic reactions: electrocyclic, cycloaddition, sigmatropic, chelotropic and group transfer reactions. Theoretical models of pericyclic reactions: TS aromaticity method (Dewar- Zimmerman approach), FMO method and Correlation diagram method (Woodward- Hoffmann approach). Woodward- Hoffmann selection rules for electrocyclic, cycloaddition and sigmatropic reactions. Stereochemistry of Diels- Alder reactions and regioselectivity. Cope and Claison rearrangements. Stereochemistry of cope rearrangement and valence tautomerism. 1, 3- dipolar cycloaddition reactions and *ene* reactions.

Unit 5: Photochemistry of Organic Compounds (9 h)

Photochemical excitation of molecules, spin multiplicity, Jablonski diagram, photosensitization, and quenching. Photochemistry of carbonyl compounds: Norrish type- I cleavage of acyclic, cyclic and β, γ- unsaturated carbonyl compounds, β-cleavage, γ-hydrogen abstraction: Norrish type- II cleavage, photo reduction, photoenolization. Photocyclo- addition of ketones with unsaturated compounds: Paterno-Büchi reaction, photodimerization of α, β- unsaturated ketones, Photo rearrangemets: Photo –Fries, di- π-methane, lumi ketone, oxa di- π- methane rearrangements.Barton and Hoffmann- Loeffler- Freytag reactions.Photo isomerization and dimerization of alkenes, photo isomerization of benzene and substituted benzenes, photooxygenation.

Unit 6: Chemistry of Natural Products (9 h)

Chemical classification of natural products. Classification of alkaloids based on ring structure, isolation and general methods of structure elucidation based on degradative reactions. Structures of atropine and quinine. Terpenoids - Isolation and classification of terpenoids, structure of steroids classification of steroids. Woodward synthesis of cholesterol,conversion of cholesterol to testosterone. Total synthesis of Longifolene, Reserpine, Cephalosporin. Introduction to flavonoids and anthocyanins (Structures only)

References:

1. M. B. Smith and J. March, March's Advanced Organic Chemistry, 6/e, John Wiley & Sons, 2007.
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7. S. Sankararaman, Pericyclic Reactions-A Textbook: Reactions, Applications and Theory, Wiley VCH, 2005.
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15. E. Corey and I.M. Chang, Logic of Chemical Synthesis, John Wiley, New York, 1989.

16. I. L. Finar, Organic Chemistry Vol 2: Stereochemistry and the Chemistry of Natural Products, 5/e, Pearson, 2006.
17. N. R.Krishnaswamy, Chemistry of Natural Products: A Laboratory Hand Book, 2/e, Universities Press.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER II

SJCHE2C08 - ELECTROCHEMISTRY, SOLID STATE CHEMISTRY AND STATISTICAL THERMODYNAMICS (3 Credits, 54h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the basic principles of ionic equilibria and electrochemistry	To develop the ability for applying the principles of chemistry.	U	F	9	-
CO2	To apply the basic principles of electrochemistry to electrochemical cells and fuel cells	To develop the ability for applying the principles of chemistry.	A	C	9	-
CO3	To understand the basic principles of crystal symmetry, stoichiometry and defects.	To be exposed to the different processes used in industries and their applications	U	C	9	-
CO4	To analyse the electronic , optical and magnetic properties of solids..	To develop the ability for applying the principles of chemistry.	Z	C	9	-
CO5	To understand the fundamental concepts of statistical mechanics.	To develop the ability for applying the principles of chemistry.	U	C	9	-
CO6	To evaluate partition functions and thermodynamic properties of gases.	To develop the ability for applying the principles of chemistry	E	C	9	-

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Ionic Interaction & Equilibrium Electrochemistry (9h)

The nature of electrolytes, Ion activity, Ion-ion and ion-solvent interaction, The electrical potential in the vicinity of an ion, Electrical potential, and thermodynamic functions. The Debye-Hückele quation,Limiting and extended forms of the Debye-Hückel equation, Applications of the Debye-Hückel equation for the determination of thermodynamic equilibrium constants and to calculate the effect of ionic strength on ion reaction rates in solution.

Origin of electrode potentials-half cell potential-standard hydrogen electrode, reference electrodes- electrochemical series, applications- cell potential, Nernst equation for electrode and cell potentials, Nernst equation for potential of hydrogen electrode and oxygen electrode- thermodynamics of electrochemical cells, efficiency of electrochemical cells and comparison with heat engines. Primary cells (Zn, MnO_2) and secondary cells (lead acid, Ni-Cd and Ni-MH cells), electrode reactions, potentials and cell voltages, advantages and limitations three types of secondary cells.

Fuel cells; polymer electrolyte fuel cell (PEMFCs), alkaline fuel cells (AFCs), phosphoric acid fuel cells (PAFCs), direct methanol fuel cells, electrode reactions and potentials, cell reactions and cell voltages, advantages and limitations of four types of fuel cells.

Unit 2: Dynamic Electrochemistry (9h)

Electrical double layer-electrode kinetics of electrode processes, the Butler-Volmer equation-The relationship between current density and overvoltage, the Tafel equation. Polarization: electrolytic polarization, dissolution and deposition potentials, concentration polarization; Overvoltage: hydrogen overvoltage and oxygen overvoltage. decomposition potential and overvoltage, individual electrode over voltages and its determination, metal deposition over voltage and its determination, theories of hydrogen overvoltage, the catalytic theory, the slow discharge theory, the electrochemical theory. Principles of polarography, dropping mercury electrode, the half wave potential.

UNIT 3: Solid State – I (9h)

Crystal symmetry: Symmetry elements and symmetry operations, mathematical proof for the non-existence of 5-fold axis of symmetry, crystal systems, Bravais lattices and crystal classes, Crystallographic point groups - Schönflies& Hermann– Mauguin

notations, Stereographic projections of the 27 axial point groups, translational symmetry elements & symmetry operations - screw axes and glideplanes, introduction to space groups.

Bragg's law and applications, lattice planes and Miller indices, *d*-spacing formulae, crystal densities and unit cell contents.

Imperfections in solids - point, line and plane defects, non-stoichiometry.

UNIT 4: Solid State – II (9h)

Electronic structure of solids: free electron theory, band theory & Zone theory, Brillouin zones; Electrical properties: electrical conductivity, Hall effect, dielectric properties, piezo electricity, ferro-electricity and ionic conductivity. Superconductivity- Meissner effect, brief discussion of Cooper theory of superconductivity. Optical properties: photo conductivity, luminescence, colour centers, lasers, refraction & birefringence. Magnetic properties: diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism & ferrimagnetism. Thermal properties - thermal conductivity & specific heat

Unit 5: Statistical Thermodynamics- I (9h)

Fundamentals: concept of distribution, thermodynamic probability and most probable distribution, ensembles, statistical mechanics for systems of independent particles and its importance in chemistry. Thermodynamic probability & entropy, idea of microstates and macrostates, statistical weight factor (g), Sterling approximation, and Maxwell-Boltzmann statistics. The molecular partition function and its relation to the thermodynamic properties, derivation of third law of thermodynamics, equilibrium-constant &equi-partition principle in terms of partition functions, relation between molecular & molar partition functions, factorisation of the molecular partition function into translational, rotational, vibrational and electronic parts, the corresponding contributions to the thermodynamic properties; Evaluation of partition functions and thermodynamic properties for ideal mono-atomic and diatomic gases.

Unit 6: Statistical Thermodynamics- II (9h)

Heat capacities of solids - classical and quantum theories, Einstein's theory of atomic crystals and Debye's modification.

Quantum Statistics: Bose-Einstein distribution law, Bose-Einstein condensation, application to liquid helium. Fermi - Dirac distribution law, application to electrons in metals; Relationship between Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics.

References (For Units 1-4)

1. D. R. Crow, *Principles and Applications of Electrochemistry*, Chapman and Hall London, 1979.
2. J.O.M. Bockrisand A.K.N. Reddy, *Modern Electrochemistry, Vol. I and II*, Kluwer Academic / Plenum Publishers, 2000.
3. Carl. H. Hamann, A. Hamnett, W.Vielstich, *Electrochemistry 2nd edn*. , Wiley-VCH, 2007.
4. Philip H Reiger, *Electrochemistry 2nd edn*. , Chapman & Hall, 1994.
5. Praveen Tyagi, *Electrochemistry*, Discovery Publishing House, 2006.
6. D.A. McInnes, *The Principles of Electrochemistry*, Dover publications, 1961.
7. L.V. Azaroff, *Introduction to Solids*, McGraw Hill, NY, 1 960.
8. A.R. West, *Basic Solid State Chemistry 2nd edn.* , John Wiley & Sons, 1999.
9. A.R. West, *Solid State Chemistry & its Applications*, John Wiley & Sons, 2003 (Reprint2007).
10. Charles Kittel, *Introduction to Solid State Physics, 7th edn*, John Wiley & Sons, 2004 (Reprint2009).
11. Mark Ladd, *Crystal Structures: Lattices & Solids in Stereo view*, Horwood, 1999.
12. Richard Tilley, *Crystals & Crystal Structures*, John Wiley & Sons, 2006.
13. C. Giacovazzo (ed.) *Fundamentals of Crystallography 2nd edn* ., Oxford Uty. Press, 2002.
14. Werner Massa, *Crystal Structure Determination 2nd edn*. , Springer2004.
15. N.B. Hanna, *Solid state Chemistry,* PrenticeHall.

For Units 5 & 6

1. G.S. Rush Brooke, Statistical mechanics, Oxford UniversityPress.
2. T.L. Hill, Introduction to statistical thermodynamics, Addison Wesley.
3. K. Huary, Statistical mechanics, Thermodynamics and Kinetics, JohnWiley.
4. O.K.Rice, Statistical mechanics, Thermodynamics and Kinetics, Freeman and Co.
5. F.C. Andrews, Equilibrium statistical mechanics, John Wiley and sons, 1963.
6. M.C. Guptha,Statistical Thermodynamics, Wiley eastern Ltd.,1993.

M.Sc. CHEMISTRY – SEMESTER I &II

SJCHE1L01 & SJCHE2L04 – INORGANIC CHEMISTRY PRACTICALS– I & II

(3 Credits)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the basic concepts of intergroup seperation.	To develop skills in the proper handling of instruments and chemicals	U	P	Nil	9
CO2	To familiarize the students with reactions of rare elements.	. To develop skills in the proper handling of instruments and chemicals	A	P	Nil	9
CO3	To gain expertise in preparation of standard solutions.	. To develop skills in the proper handling of instruments and chemicals	A	P	Nil	10
CO4	To acquire skills in quantitative colorimetric analysis.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	10
CO5	To apply the acquired skills to analyse quality of potable water and food samples.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	5

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

UNIT 1: Inorganic Cation Mixture Analysis

Separation and identification of four metal ions of which two are less familiar elements like W, Se Te, Mo, Ce, Th, Ti, Zr, V, U, and Li. (Eliminating acid radicals not present). Confirmation by spot tests.

UNIT 2: Volumetric Analysis

Volumetric Determinations using:

a) EDTA (Al, Ba, Ca, Cu, Fe, Ni, Co, hardness of water)
b) Cerimetry (Fe^{2+},nitrite)
c) Potassium Iodate (Iodide,Sn^{2+})

UNIT 3: Colorimetric Analysis

Colorimetric Determinations of metal ions Fe, Cr, Ni, Mn, and Ti.

References

1. G.H. Jeffery, J. Basseett, J. Mendham andR.C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, 5th Edition, ELBS, 1989.
2. D.A. Skoog and D.M. West, *Analytical Chemistry, an Introduction*, 4th Edition, CBS Publishing Japan Ltd., 1986.
3. E.J. Meehan, S. Bruckenstein and I.M. Kolthoff and E.B. Sandell, *Quantitative Chemical Analysis*, 4th Edition, The Macmillan Company,1969.
4. R.A. Day (Jr.) and A.L. Underwood, *Quantitative Analysis*, 6th Edition, Prentice Hall of India, 1993.

M.Sc. CHEMISTRY – SEMESTER I &II

SJCHE1L02 & SJCHE2L05 – ORGANIC CHEMISTRY PRACTICALS– I & II

(3 Credits)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To practice various purification techniques.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	9
CO2	To prepare organic compounds by multistage methods.	. To develop skills in the proper handling of instruments and chemicals	A	P	Nil	9
CO3	To enable functional group analysis.	. To develop skills in the proper handling of instruments and chemicals	A	P	Nil	10
CO4	To analyse organic binary mixture.	To develop skills in the proper handling of instruments and chemicals	Z	P	Nil	10
CO5	To determine the physical constants of organic compounds.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	5
CO6	To apply organic qualitative analysis by microscale techniques.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	5

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Unit 1: Laboratory Techniques

Methods of Separation and Purification of Organic Compounds: fractional, steam and low-pressure distillations, fractional crystallization and sublimation.

Unit 2: Separation and identification of the components of organic binary mixtures.
(Microscale analysis is preferred)

Analysis of about ten binary mixtures, some of which containing compounds with more than one functional group. Separation and identification of a few ternary mixtures.

Unit 3: Organic preparations-double stage (minimum six) and three stage (minimum two)

References:

1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, 5/e, Pearson, 1989.
2. Shriner, FusonandCartin, Systematic Identification of Organic Compounds, 1964.
3. Fieser, Experiments in Organic Chemistry, 1957.
4. Dey, Sitaraman and Govindachari, A Laboratory Manual of Organic Chemistry, 3rdEdition, 1957.
5. P.R. Singh, D.C. Gupta, and K.S. Bajpal, Experimental Organic Chemistry, Vol. I and II, 1980.
6. Vishnoi, Practical Organic Chemistry.
7. Pavia, Kriz, Lampman, and Engel, A Microscale Approach to Organic Laboratory Techniques, 5/e, Cengage, 2013.
8. Mohrig, Hammond and Schatz, Techniques in Organic Chemistry: Miniscale, Standard Taper Microscale and Williamson Microscale, 3/e, W. H. Freeman and Co., 2010.

M.Sc. CHEMISTRY – SEMESTER I & II

SJCHE1L03 & SJCHE2L06 – PHYSICAL CHEMISTRY PRACTICALS – I &II

(3 Credits)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To determine the molar heat of solution of a substrate.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	9
CO2	To determine phase diagram of a simple eutectic system.	. To develop skills in the proper handling of instruments and chemicals	A	P	Nil	9
CO3	. To determine phase diagram of a binary solid system forming a compound.	. To develop skills in the proper handling of instruments and chemicals	Z	P	Nil	10
CO4	To determine molar refractions of pure liquids..	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	10
CO5	To apply the principles of viscosity to determine molecular weight of a polymer.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	5

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SECTION A

Unit 1: Solubility and Heat of solution (minimum 2 experiments)

1. Determination of molar heat of solution of a substance (e.g., ammonium oxalate, succinic acid) from solubility data - analytical method and graphical method

Unit 2: Phase Equilibria (minimum 3 experiments)

1.(a) Determination of phase diagram of a simple eutectic system (e.g., Biphenyl, Naphthalene- Diphenyl amine) (b) Determination of the composition of a binary solid mixture.

2.Determination of phase diagram of a binary solid system forming a compound (e.g., Naphthalene –m-dinitrobenzene).

Unit 3: Viscosity (minimum 2 experiments)

1.Viscosity of mixtures - Verification of Kendall's equation (e.g., benzene-nitrobenzene,water-alcohol).

2.Determination of molecular weight of a polymer (e.g., polystyrene)

Unit 4: Distribution Law (minimum 3 experiments)

1.Determination of distribution coefficient of I2 between CCl4 and H2O.

2.Determination of equilibrium constant of KI + I2 =KI3

3.Determination of concentration of KI solution.

SECTION B

Unit 5: Refractometry (minimum 3 experiments)

1.Determination of molar refractions of pure liquids (e.g:water, methanol, ethanol, chloroform, carbon tetrachloride,glycerol)

2.Determination of the composition of liquid mixtures (e.g., alcohol-water, glycerol-water)

3.Determination of molar refraction and refractive index of a solid.

Unit 6: Conductivity (minimum 4 experiments)

1.Determination of equivalent conductance of a weak electrolyte (e.g., acetic acid), verification of Ostwald's dilution law and calculation of dissociation constant.

2.Determination of solubility product of a sparingly soluble salt (e.g., AgCl,$BaSO_4$)

3.Conductometric titrations

(a)HCl vs NaOH

(b)(HCl + CH_3COOH) vs NaOH

4.Determination of the degree of hydrolysis of aniline hydrochloride

Unit 7: Potentiometry (minimum 3 experiments)

1.Potentiometric titration: HCl vs NaOH, CH_3COOH vs NaOH

2.Redox titration: KI vs $KMnO_4$, $FeSO_4$ vs $K_2Cr_2O_7$

3.Determination of dissociation constant of acetic acid by potentiometric titration

4.Determination of pH of weak acid using Potentiometry

5.Determination of pH of acids and bases using pHmeter

Reference:

1. A. Finlay, Practical Physical Chemistry, Longman's Green &Co.

2. J.B. Firth, Practical Physical Chemistry, Read Books (Reprint2008).

3. A.M. James, Practical Physical Chemistry, Longman, 1974.

4. F.Daniel,J.W.Williams,P.Bender,R.A.Alberty,C.D.CornwellandJ.E.Harriman,

Experimental Physical Chemistry, McGraw Hill, 1970.

5. W.G. Palmer, Experimental Physical Chemistry, 2nd Edition, Cambridge University Press, 1962.

6. D.P. Shoemaker and C.W. Garland, Experimental Physical Chemistry, McGraw-Hill.

7. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publications 1989.

8. B. Viswanathan & R.S. Raghavan, Practical Physical Chemistry, Viva Books, 2009.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III

SJCHE3C09 - MOLECULAR SPECTROSCOPY (4 Credits, 72h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the basics of microwave spectroscopy	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO2	To understand the basics of infrared, raman, and electronic spectroscopy	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO3	To analyse the structure of organic compounds using infrared and electronic spectroscopy	To develop the ability for applying the principles of chemistry.	Z	P	9	Nil
CO4	To understand the basics of NMR and ESR spectroscopy	To develop the ability for applying the principles of chemistry.	U	F	18	Nil
CO5	To analyse the structure of organic compounds using NMR spectroscopy	To develop the ability for applying the principles of chemistry.	Z	P	18	Nil
CO6	To apply the mass spectrometry for the structure elucidation of organic compounds	To develop the ability for applying the principles of chemistry.	A	P	9	Nil

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*F-factual, C-conceptual, P-practical/procedural

Unit 1: Basic Aspects and Microwave Spectroscopy - Theory only (9h)

Electromagnetic radiation & it's different regions, interaction of matter with radiation and its effect on the energy of a molecule, factors affecting the width and intensity of spectral lines. Microwave spectroscopy : Rotation spectra of diatomic and poly atomic molecules - rigid and non-rigid rotator models, asymmetric, symmetric and spherical tops, isotope effect on rotation spectra, Stark effect, nuclear and electron spin interactions, rotational transitions and selection rules, determination of bond length using microwave spectral data.

Unit 2: Infrared, Raman and Electronic Spectroscopy - Theory only (9h)

Vibrational spectroscopy: Normal modes of vibration of a molecule, vibrational spectra of diatomic molecules, anharmonicity, Morse potential, fundamentals, overtones, hot bands, combination bands, difference bands, vibrational spectra of polyatomic molecules, Vibration-rotation spectra of diatomic and polyatomic molecules, spectral branches -P, Q & R branches.

Raman spectroscopy: Classical and Quantum theory of Raman Effect Pure rotational & pure vibrational Raman spectra, vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Introduction to Resonance Raman spectroscopy (basics only).

Electronic Spectroscopy: Characteristics of electronic transitions – Vibrational coarse structure, intensity of electronic transitions, Franck - Condon principle, types of electronic transitions, Dissociation and pre-dissociation, Ground and excited electronic states of diatomic molecules, Electronic spectra of polyatomic molecules, Electronic spectra of conjugated molecules.

Unit 3: Magnetic Resonance Spectroscopy – I - Theory only (9h)

NMR: Quantum mechanical description of Energy levels-Population of energy-Transition probabilities using ladder operators, Nuclear shielding, Chemical shift, Spin-Spin coupling and splitting of NMR signals, Quantum mechanical Description- AX and AB NMR pattern. Effect of Relative magnitudes of J (Spin-Spin coupling) and Chemical Shift on the spectrum of AB type molecule. Karplus relationship. Nuclear Overhauser Effect- FT NMR- Pulse sequence for T1 and T2 (Relaxation) measurements. 2D NMR COSY

Unit 4: Magnetic Resonance Spectroscopy – II - Theory only (9h)

Electron Spin Resonance: Quantum mechanical description of electron spin in a magnetic field, Energy levels-Population- Transition probabilities using Ladder operators, g factor-

hyperfine interaction, Mc Connell Relation, Equivalent and non-equivalent nucleus, g anisotropy, Zero field splitting -Kramer's theorem.

Mossbauer Spectroscopy: The Mossbauer Effect, hyperfine interactions, isomer shift, electric quadruple and magnetic hyperfine interactions.

UNIT 5: Electronic & Vibrational Spectroscopy in Organic Chemistry (9h)

UV-Visible spectroscopy: Factors affecting the position and intensity of electronic absorption bands – conjugation, solvent polarity and steric parameters. Empirical rules for calculating λmax of dienes, enones and benzene derivatives.

Optical Rotatory Dispersion and Circular Dichroism: Linearly and circularly polarized lights, circular birefringence, elipticity and circular dichroism, ORD and Cotton effect. Octant rule andaxial haloketone rule for the determination of conformation and configuration of 3-methyl cyclohexanone and cis- and trans-decalones. CD curves.

Infrared Spectroscopy: Functional group and finger print regions, Factors affecting vibrational frequency: Conjugation, coupling, electronic, steric, ring strain and hydrogen bonding. Important absorption frequencies of different class of organic compounds-hydrocarbons, alcohols, thiols, carbonyl compounds, amines, nitriles.

UNIT 6: NMR Spectroscopy in Organic Chemistry - I (9h)

1HNMR: Chemical shift, factors influencing chemical shift, anisotropic effect. Chemical shift values of protons in common organic compounds, chemical, magnetic and stereochemical equivalence. Enantiotopic, diasteriotopic and homotopic protons. Protons on oxygen and nitrogen. Quadrapole broadening. Spin – spin coupling, types of coupling, coupling constant, factors influencing coupling constant, effects of chemical exchange, fluxional molecules, hindered rotation on NMR spectrum, first order and non-first order NMR spectra.

UNIT 7: NMR Spectroscopy in Organic Chemistry - II (9h)

Simplification of NMR spectra: double resonance, shift reagents, increased field strength, deuterium labelling. NOE spectra, heteronuclear coupling. Introduction to COSY, HMBC, HMQC spectra.

13C NMR: General considerations, comparison with PMR, factors influencing carbon chemical shifts, carbon chemical shifts and structure-saturated aliphatics, unsaturated

aliphatics, carbonyls, and aromatics. Off-resonance and noise decoupled spectra, Introduction to DEPT, INEPT, INADEQUATE.

UNIT 8: Mass Spectrometry and Spectroscopy for Structure Elucidation (9h)

Mass Spectrometry: Basic concept of EIMS. Molecular ion and metastable ion peaks, isotopic peaks. Molecular weight and molecular formula. Single and multiple bond cleavage, rearrangements - McLafferty rearrangements. Fragmentation pattern of some common organic compounds – saturated and unsaturated hydrocarbons, ethers, alcohols, aldehydes and ketones, amines and amides. High resolution mass spectrometry, index of hydrogen deficiency, Nitrogen rule and Rule of Thirteen. Ionization techniques. FAB spectra.

Structural determination of organic compounds using spectroscopic techniques (Problem solving approach)

References: For Units 1, 2, 3 & 4

1. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1962.
2. C.N. Banwell& E. M. McCash, Fundamentals of Molecular Spectroscopy, Tata McGraw Hill,New Delhi,1994.
3.Thomas Engel, Quantum Chemistry & Spectroscopy, Pearson education, 2006.
4.P. Atkins & J. De Paula, Atkins's Physical Chemistry, 8th Edition, W.H. Freeman & Co., 2006.
5.D.A. McQuarrie and J.D. Simon, Physical Chemistry - A Molecular Approach, University Science Books, 1997.
6.D.N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques, UniversityPress, 2000.
7.R.S. Drago, Physical methods for Chemists, Second edition, Saunders College Publishing 1977 (For NMR and EPR,Mossbauer)
8.Gunther, NMR Spectroscopy:Basic Principles, Concepts and Applications in Chemistry,2/e,– John Wiley
9. Ferraro, Nakamoto and Brown, Introductory Raman Spectroscopy, 2/e, Academic Press, 2005.

For Units 5, 6, 7 & 8

1. Lambert, Organic Structural Spectroscopy,2/e,Pearson
2. Silverstein, Spectrometric Identification of Organic Compounds, 6/e,John Wiley

3. Pavia, Spectroscopy, 4/e, Cengage
4.Jag Mohan, Organic Spectroscopy: Principles and Applications,2/e,Narosa
5. Fleming, Spectroscopic Methods in Organic Chemistry, 6/e, McGraw-Hill
6. P S Kalsi, Spectroscopy of organic compounds, New Age International,2007 William Kemp, Organic Spectroscopy, 3e, Palgrave, 2010.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III

CHE3C10 - ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY (4 Credits, 54h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the role of metal ions in biological systems.	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO2	To understand the significance of enzymes in biological systems.	To develop the ability for applying the principles of chemistry.	U	C	9	Nil
CO3	To understand the applications of organometallic compounds.	To be exposed to the different processes used in industries and their applications	A	C	9	Nil
CO4	To analyse bonding pattern and stability of organometallic compounds.	To develop the ability for applying the principles of chemistry.	Z	C	9	Nil
CO5	To understand the reactivity and reactions given by organometallic compounds.	To develop the ability for applying the principles of chemistry.	U	C	9	Nil
CO6	To understand the stability of organometallic compounds using 18-electron rule.	To develop the ability for applying the principles of chemistry.	U	C	9	Nil

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*F-factual, C-conceptual, P-practical/procedural

Unit 1: Introduction to Organometallic Chemistry (9h)

Historical background. Classification and nomenclature. Alkyls and aryls of main group metals. Organometallic compounds of transition metals. The 18-electron rule, electron counting by neutral atom method and oxidation state method. The 16-electron rule.

Metal carbonyls- Synthesis, structure, bonding and reactions. Nitrosyl, dihydrogen and dinitrogen complexes. Transition metal to carbon multiple bond-metal carbenes and carbines.

Unit 2: Organometallic Compounds of Linear and Cyclic π-Systems (9h)

Transition metal complexes with linear π- systems- Hapticity. Synthesis, structure, bonding and properties of complexes with ethylene, allyl, butadiene and acetylene. Complexes of cyclic π- systems-Synthesis, structure, bonding and properties of complexes with cyclobutadiene, C_5H_5- C_6H_6, $C_7H_7^+$ and $C_8H_8^{2-}$. Fullerene complexes. Fluxional organometallics.

Unit 3: Organometallic Reactions and Catalysis (9h)

Organometallic reactions- ligand dissociation and substitution- Oxidative addition and reductive elimination. Insertion reactions involving CO and alkenes. Carbonylation by Collman`s reagent. Electrophilic and Nucleophilic attack on coordinated ligand.

Homogeneous and heterogeneous catalysts. Homogeneous catalysis by organometallic compounds: Hydrogenation by Wilkinson`s catalyst, Hydroformylation, Wacker process, Monsanto acetic acid process, Cativa process and olefin metathesis.

Heterogeneous catalysis by organometalic compounds: Ziegler-Natta polymerizations, Fischer- Tropsch process and water gas shift reaction.

Unit 4: Metal Clusters (9h)

Metal-Metal bond and metal clusters. Bonding in metal-metal single, double, triple and quadruple bonded non-carbonyl clusters. Carbonyl clusters-electron count and structure of clusters. Wade-Mingos-Lauher rules. Structure and isolobal analogies. Carbide clusters. Polyatomic Zintl anions and cations. Chevrel phases.

Unit 5: Bioinorganic Chemistry-I (9h)

Occurrence of inorganic elements in biological systems- bulk and trace metal ions.

Emergence of bioinorganic chemistry. Coordination sites in biologically important ligands. Ion transport across membranes. Role of alkali metal ions in biological systems. The sodium/potassium pump. Structural role of calcium. Storage and transport of metal ions-ferritin, transferrin and siderophores. Oxygen transport by heme proteins-hemoglobin and

myoglobin-structure of the oxygen binding site-nature of heme-dioxygen binding-cooperativity. Hemerythrin and hemocyanin.

Unit 6: Bioinorganic Chemistry-II (9h)

Metallo enzymes and electron carrier metallo proteins. Iron enzymes: Cytochrome P-450, catalase and peroxidase. Copper enzymes: Oxidase, superoxide dismutase and tyrosinase. Lewis acid role of Zn (II) and Mn(II) containing enzymes. Carboxypeptidase. Vitamin B12 and coenzymes. Chlorophil II- Photosystem I and II. Nitrogen fixation-Nitrogenases. Anticancer drugs.

References:

1. N.N. Greenwood and A. Earnshaw, Chemistry of Elements, 2/e, Elsevier Butterworth-Heinemann, 2005.
2. J.E. Huheey, E.A. Keiter, R.L. Keiter. O.K. Medhi, Inorganic Chemistry, principles of structure and reactivity, Pearson Education, 2006.
3. G.L. Miessler, D.A.Tarr, Inorganic Chemistry, Pearson, 2010.
4. D.F. Shriver, P.W. Atkins, Inorganic Chemistry, Oxford University Press,2002
5. William W Porterfield, Inorganic Chemistry-A unified approach, Academic Press, 2005.
6. Keith F Purcell, John C Kotz, Inorganic Chemistry, Cengage Learning, 2010.
7. James E House, Inorganic Chemistry, Academic Press, 2008.
8. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, Wiley Student Edition, 2006.
9. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley.
10. R.C. Mehrothra and A. Singh, Organometallic Chemistry, A Unified Approach, Wiley Eastern.
11. P.Powell, Principles of Organometallic Chemistry, ELBS.
12. B.D.Gupta and A.J.Elias, Basic Organometallic Chemistry, Concepts, Synthesis and Applications, Universities Press, 2010.
13. Piet W.N. M.van Leeuwen, Homogeneous Catalysis, Springer, 2010.S.J. Lippard and J.M.Berg, Principles of Bioinorganic Chemistry, University ScienceBooks.
14. I. Bertini, H.B. Grey, S.J. Lippard and J.S.Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., 1998.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III

CHE3C11 - REAGENTS AND TRANSFORMATIONS IN ORGANIC CHEMISTRY
(4 Credits, 54h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the oxidation reactions in organic chemistry.	To be exposed to the different processes used in industries and their applications	U	F	9	Nil
CO2	To understand various types of polymerization.	To develop the ability for applying the principles of chemistry.	U	C	9	Nil
CO3	To apply the principles of reduction and various coupling reactions in organic synthesis.	To be exposed to the different processes used in industries and their applications	A	C	9	Nil
CO4	To analyse natural and artificial supramolecular systems.	To develop the ability for applying the principles of chemistry.	Z	C	9	Nil
CO5	To analyse the strategy of peptide synthesis.	To develop the ability for applying the principles of chemistry.	Z	C	9	Nil
CO6	To understand the use of important synthetic reagents for organic reactions.	To be exposed to the different processes used in industries and their applications	U	C	9	Nil

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Unit 1: Oxidations (9h)

Oxidation of alcohols to carbonyls using DMSO, oxoammonium ions and transition metal oxidants (chromium, manganese, iron, ruthenium). Epoxydation of alkenes by peroxy acids, Sharpless asymmetric epoxidation, Jacobsen epoxidation, dihydroxylation of alkenes using permanganate ion and osmium tetroxide, Prévost and Woodward dihydroxylations, Sharpless asymmetric dihydroxylation. Allylic oxidation with CrO3, Pyridine reagent. Oxidative cleavage of alkenes to carbonyls using O3. Oxidative decarboxylation, Riley reaction, Baeyer Villiger oxidation, Dess Martin oxidation, Swern oxidation, hydroboration oxidation.

Unit 2: Reductions (9h)

Catalytic hydrogenation of alkenes and other functional groups (heterogeneous and homogeneous), Noyori asymmetric hydrogenation, hydrogenolysis. Liquid ammonia reduction with alkali metals. Metal hydride reductions. Reduction of carbonyl group with hydrazine, p-tosylhydrazine, diimide and semicarbazide. Clemmensen reduction, Birch reduction. Wolff Kishner reduction, Bouveault Blanc reduction, MPV reduction, hydroboration, Pinacol coupling, McMurry coupling, Shapiro reaction.

Unit 3: Synthetic Reagents (9 h)

Synthetic applications of Crown ethers, β-cyclodextrins, PTC, ionic liquids, Baker's yeast, NBS, LDA, LiAlH4, LiBH4, DIEA, BuLi, diborane, 9-BBN, t-butoxycarbonylchloride, DCC, Gilman's reagent, lithium dimethyl cuprate, tri-n-butyltinhydride, 1,3-dithiane, trimethyl silyl chloride, Pb(OAc)4, ceric ammonium nitrate, DABCO, DMAP, DBU, DDQ, DEAD and Lindlar catalyst in organic synthesis.

Unit 4: Chemistry of Polymers (9 h)

Classification of polymers, chain, step, free-radical and ionic polymerizations. Plastics, rubbers and fibers, thermosets and thermoplastics, linear, branched, cross -linked and network polymers, block and graft copolymers.

Natural and synthetic rubbers.

Biopolymers: Primary, secondary and tertiary structure of proteins, Merrifield solid phase peptide synthesis, Protecting groups, sequence determination of peptides and proteins, Structure and synthesis of glutathione, structure of RNA and DNA, structure of cellulose and starch, conversion of cellulose to rayon.

Unit 5: Heterocyclic chemistry and supramolecular chemistry (9 h)

Aromatic and nonaromatic heterocyclics. Structure, synthesis and reactions of a few heterocyclics- aziridine, oxirane, indole, pyridine, quinolone, imidazole. Synthesis of uracil, thymine, adenine and guanine

Supramolecular Chemistry: Basic concepts and terminology. Molecular recognition: Molecular receptors for different types of cations, anions and neutral molecules, design of coreceptors and multiple recognition. Strong, weak and very weak Hydrogen bonds. Use of H bonds in in crystal-engineering and molecular recognition. Supramolecular reactivity and catalysis. Supramolecular photochemistry and examples for supramolecular devices

Unit 6: Molecular Rearrangements and Transformations (9h)

Rearrangements occurring through carbocations, carbanions, carbenes and nitrenes such as Wagner-Meerwein, Demjanov, dienone-phenol, benzyl-benzilic acid, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Fries, Bayer-Villiger, Wittig, Orton, and Fries rearrangements. Peterson reaction, Woodward and Prevost hydroxylation reactions. Heck, Negishi, Sonogashira, Stille, and Suzuki coupling reactions (mechanism only)

References:

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3. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, 4/e, Cambridge UniversityPress.
4. R. R. Carey and R. J. Sundburg, Advanced Organic Chemistry, Part B, 5/e, Springer, 2007.
5. M. B. Smith, J. March, March's Advanced Organic Chemistry, 6/e, John Wiley & Sons, 2007.
6. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 2/e, Oxford University Press, 2012.
7. J. J. Li, Name Reactions, 4/e, Springer, 2009.
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9. G. Odiyan, Principles of Polymerisation, 4/e, Wiley, 2004.
10. V.R. Gowariker and Others, Polymer Science, Wiley EasternLtd.
11. I.L. Finar, Organic Chemistry, Vol. II, 5/e, ELBS, 1975.
12. J. A. Joules and K. Mills, Heterocyclic Chemistry, 4/e, Oxford University Press, 2004.
13. T. L. Gilchrist, Heterocyclic Chemistry, 3/e, Pearson, 1997.

14. T. H. Lowry and K. S. Richardson, Mechanism and Theory in Organic Chemistry, 3/e Addison-Wesley, 1998.
15. F. Vogtle, Supramolecular Chemistry, John Wiley & Sons, Chichester, 1991.
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M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III CHE3E01 - SYNTHETIC ORGANIC CHEMISTRY (ELECTIVE)

(4 Credits, 54h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the chemistry of carbonyl condensation reactions.	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO2	To understand the chemistry of fused and higher ring heterocyclics..	To develop the ability for applying the principles of chemistry.	U	C	9	Nil
CO3	To understand the basic principle of multistep synthesis.	To be exposed to the different processes used in industries and their applications	U	C	9	Nil
CO4	To apply metal catalyzed coupling reaction in organic synthesis..	To be exposed to the different processes used in industries and their applications	A	C	9	Nil
CO5	To apply organometallic and organo-nonmetallic reagents in organic synthesis.	To be exposed to the different processes used in industries and their applications	A	C	9	Nil
CO6	To apply reagents for oxidation reduction reactions	To be exposed to the different processes used in industries and their applications	A	C	9	Nil

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Reagents for Oxidation and Reduction (9h)

Reagents for oxidation and reduction: Oxone, IBX, PCC, osmium tetroxide, ruthenium tetroxide, selenium dioxide, molecular oxygen (singlet and triplet), peracids, hydrogen peroxide, aluminum isopropoxide, periodic acid, lead tetraacetate. Wacker oxidation, TEMPO oxidation, Swern oxidation, Woodward and Prevost hydroxylation, Sharpless asymmetric epoxidation.
Catalytic hydrogenations (heterogeneous and homogeneous), metal hydrides, Birch reduction, hydrazine and diimide reduction.

Unit 2: Organometallic and Organo-nonmetallic Reagents (9h)

Synthetic applications of organometallic and organo-nonmetallic reagents. Reagents based on chromium, nickel, palladium, silicon, and born, Gilman reagent, phase transfer catalysts, hydroboration reactions, synthetic applications of alkylboranes. Gilman's reagent, Tri -n-butyl tin hydride, Benzene TricarbonylChromium

Unit 3: Chemistry of Carbonyl Compounds (9h)

Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides, amides. Substitution at α-carbon, aldol and related reactions, Claisen, Darzen, Dieckmann, Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Reaction with phosphorous and sulfurylides.
Protecting groups, functional group equivalents, reversal of reactivity (Umpolung), Introduction to combinatorial chemistry.

Unit- 4. Coupling Reactions (9h)

Coupling Reactions: PalladiumCatalysts for C-N and C-O bond formation, Palladium catalyzed amine arylation (Mechanism and Synthetic applications). Sonogashira cross coupling reaction (Mechanism, Synthetic applications in cyclic peptides) Stille carbonylative cross coupling reaction (Mechanism and synthetic applications). Mechanism and synthetic applications of Negishi, Hiyama, Kumada, Heck and Suzuki-Miyaura coupling reactions.

Unit 5: Multi step Synthesis (9h)

Multi step Synthesis: Synthetic analysis and planning, Target selection, Elements of a Synthesis (Reaction methods, reagents, catalysts, solvents, protective groups for hydroxyl,

amino, Carbonyl and carboxylic acids, activating groups, leaving groups synthesis and synthetic equivalents. Types of selectivities (Chemo, regio, stereo selectivities) synthetic planning illustrated by simple molecules, disconnections and functional group interconversions, umpolung reactions and use in synthesis. Introduction to retrosynthetic analysis, Synthesis of longifolene, Corey lactone, Djerassi Prelog lactone

Unit 6: Retro Synthetic Analysis and Heterocyclics (9h)

Retrosynthesis: General principles of retrosynthetic analysis. Synthons and reagents, donor and acceptor synthons, umpolung, protecting group chemistry and functional group interconversions. One group and two group C-X and C-C disconnections, functional group transposition. Examples for a few retrosynthetic analyses- paracetamol from phenol, benzocain from toluene and propranolol from 1-naphthol.
Structure, synthesis and reactions of fused ring heterocycles: Benzofuran, Indole, Benzothiophene, Quinoline, Benzoxazole, Benzthiazole, Benzimidazole, Triazoles, Oxadiazoles and Tetrazole. Structure and synthesis of Azepines, Oxepines, Thiepins, Diazepines and Benzodiazepines Structure and synthesis (Reichstein process) of Vitamin C (Reichstein process).

References:

1. M. B. Smith, Organic Synthesis, 3/e, Academic Press, 2011.

2. S. Warren and P. Wyatt, Organic Synthesis: Strategy and Control, John Wiley

3. S. Warren: Organic Synthesis: The Disconnection Approach, JohnWiley

4. H. O. House: Modern Synthetic Reactions, W. A.Benjamin

5. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, 4/e, Cambridge UniversityPress.

6. T. W. Greene and P. G. M. Wuts: Protecting Groups in Organic Synthesis, 2nd ed., John Wiley

7. MBSmithandJ.March:AdvancedOrganicChemistry-Reactions,MechanismsandStructure, 6th ed., John Wiley

8. T. H. Lowry and K. S. Richardson: Mechanism and Theory in Organic Chemistry, 3rded.

9. R. R. Carey and R. J. Sundburg, Advanced Organic Chemistry, Part A and B, 5/e, Springer, 2007

10. A. Pross: Theoretical and Physical Principles of Organic Chemistry, JohnWiley

11. T.W. Graham Solomons: Fundamentals of Organic Chemistry, 5th ed., JohnWiley

12. I. L. Finar: Organic Chemistry Volumes 1 (6th ed.),Pearson

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M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III

SJCHE3E02: COMPUTATIONAL CHEMISTRY (ELECTIVE)

(4 Credits, 54h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the basics of quantum mechanics and computational methods	To develop the ability for applying the principles of chemistry.	U	F	12	Nil
CO2	To understand the concept of electron correlation and post HF methods	To develop the ability for applying the principles of chemistry.	U	F	12	Nil
CO3	To understand the classification of computational methods and basis sets	To develop the ability for applying the principles of chemistry.	U	F	12	Nil
CO4	To apply the computational methods for molecular simulations	To develop the ability for applying the principles of chemistry.	A	P	18	Nil

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Introduction to Computational Chemistry (9 h)

Theory, computation & modeling – Definition of terms. Need of approximate methods in quantum mechanics. Computable Quantities – structure, potential energy surfaces and chemical properties. Cost & Efficiency – relative CPU time, software & hardware. Classification of computational methods.

Unit 2: Computer Simulation Methods- I (9 h)

Introduction – molecular dynamics and Monte Carlo methods, calculation of simple thermodynamic properties - energy, heat capacity, pressure and temperature, phase space, practical aspects of computer simulation, periodic boundary conditions, Monitoring the equilibration, analyzing the results of a simulation, error estimation.

Unit 3: Computer Simulation Methods- II (9 h)

Molecular dynamics (MD) method – molecular dynamics using simple models – MD with continuous potentials, finite difference methods, choosing the time step, setting up and running a MD simulation. Monte Carlo (MC) method - calculating properties by integration, Metropolis method, random number generators, MC simulation of rigid molecules.

Unit 4: ab intio Methods in Computational Chemistry (9h)

Review of Hartree – Fock method for atoms, SCF treatment of polyatomic molecules; Closed shell systems - restricted HF calculations; Open shell systems – ROHF and UHF calculations; The Roothan – Hall equations, Koopmans theorem, HF limit & electron correlation, Introduction to electron correlation (post -HF) methods.

Unit 5: Density Functional Methods (9 h)

Introduction to density matrices, N-reprentability & V-represetability problems, Hohenberg–Kohn theorems, Kohn-Sham orbitals, Exchange correlation functionals– Thomas-Fermi-Dirac model, Local density approximation, generalised gradient approximation, hybrid functional. Comparison between DFT and HF methods.

Unit 6: Basis Set Approximation (9 h)

Hydrogen-like, Slater-type & Gaussian type basis functions, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization & diffuse basis sets, even tempered &well-tempered basis sets, contracted basis sets, Pople-style basis sets and their

nomenclature, correlation consistent basis sets, basis set truncation error, effect of choice of method/ basis set (model chemistries) on cpu time.

References:

1. C. J. Cramer, Essentials of computational Chemistry: Theories and models, John Wiley & Sons 2002.

2. Frank Jensen, Introduction to Computational Chemistry, John Wiley & Sons LTD1999.

3. J. Foresman &Aelieen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.

4. David Young, Computational Chemistry- A Practical Guide for Applying Techniques to Real- World Problems", Wiley -Interscience, 2001.

5. Errol G. Lewars, Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics, 2 nd edn, Springer2011.

6. I.N. Levine, Quantum Chemistry, 6th Edition, Pearson Education Inc., 2009.

7. P.W. Atkins & R.S. Friedman, Molecular quantum mechanics, 4th Edition, Oxford University Press, 2005.

8. W. Koch, M.C. Holthausen, "A Chemist's Guide to Density Functional Theory", Wiley-VCH Verlag2000.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER III

SJCHE3E03: GREEN AND NANOCHEMISTRY (ELECTIVE)

(4 Credits, 54h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand goals and principles of green synthesis	To develop the ability for applying the principles of chemistry.	U	F	8	Nil
CO2	To apply the green strategy in synthetic organic chemistry	To be exposed to the different processes used in industries and their applications.	A	P	12	Nil
CO3	To understand the basics of nanochemistry	To develop the ability for applying the principles of chemistry.	U	F	8	Nil
CO4	To understand the structure, properties, and applications of carbon based nanomaterials	To be exposed to the different processes used in industries and their applications.	U	P	10	Nil
CO5	To synthesise and characterize nanomaterials	To be exposed to the different processes used in industries and their applications.	Z	P	16	Nil

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit I: Introduction to green chemistry (9h)

Green chemistry-relevance and goals, Anastas' twelve principles of green chemistry - Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples.

Unit 2: Microwave mediated organic synthesis (MAOS) (9h)

Microwave activation, advantage of microwave exposure, specific effects of microwave – Neat reactions, solid supports reactions, Functional group transformations, condensations reactions, oxidations – reductions reactions, multi-component reactions.

Unit 3: Alternative synthesis, reagents and reaction conditions (9h)

Introduction, synthesis of ionic liquids, physical properties, applications in alkylation – hydroformylations , expoxidations , synthesis of ethers, Friedel-craft reactions, Diels-Alder reactions , Knoevengal condensations, Wittig reactions, Phase transfer catalyst - Synthesis– applications. A photochemical alternative to Friedel-crafts reactions - Dimethyl carbonate as a methylating agent – the design and applications of green oxidants – super critical carbon dioxide for synthetic chemistry.

Unit 4: Nanomaterials – An Introduction & Synthetic Methods (9h)

Definition of nano dimensional materials - Historical milestones - unique properties due to nanosize, Quantum dots, Classification of Nanomaterials .General methods of synthesis of nanomaterials – Hydrothermal synthesis, Solvothermal synthesis, Microwave irradiation, sol – gel and Precipitation technologies, Combustion Flame-Chemical Vapor Condensation Process, gas Phase Condensation Synthesis, Reverse Micelle Synthesis, Polymer – Mediated Synthesis, Protein Microtube – Mediated Synthesis. Synthesis of Nanomaterials using microorganisms and other biological agents, Sonochemical Synthesis, Hydrodynamic Cavitation. Inorganic nanomaterials – Typical examples –nano TiO_2/ ZnO/CdO/CdS, Organic nanomaterials – examples – Rotaxanes and Catenanes

Unit 5: Techniques for Characterisation of nanoscale materials (9h)

Principles of Atomic force microscopy (AFM), Transmission electron microscopy (TEM)-Resolution and scanning transition electron microscopy (STEM), Scanning Tunneling Microscopy (STM), Scanning near field optical microscopy (SNOM), Scanning ion

conductance microscope, scanning thermal microscope, scanning probe microscopes and surface plasmon spectroscopy.

Unit 6: Carbon Clusters and Nanostructures (9h)

Nature of carbon bond, new carbon structures. Carbon clusters: Discovery of C60, Alkali doped C60, Superconductivity in C60, Larger and smaller fullerenes. Carbon nanotubes: Synthesis, Single walled carbon nanotubes, Structure and characterization, Mechanism of formation. Chemically modified carbon nanotubes, Doping - Functionalizing nanotubes. Application of carbon nanotubes. Nanowires: Synthetic strategies, Gas phase and solution phase growth, Growth control - Properties.

References:

For Units 1, 2 & 3

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3. Green Chemistry – Designing Chemistry for the Environment – edited by Paul T. Anastas& Tracy C. Williamson. Second Edition, (1998).
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5. Green Chemistry – Environment friendly alternatives- edited by Rashmi Sanghi& M. M. Srivastava, Narora Publishing House, (2003).

For Units 4, 5 & 6

1. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, 2, Wiley –VCH, Weinheim, 2004.
2. C.P. Poole, Jr: F.J. Owens, Introduction to Nanotechnology Wiley Interscience, New Jersey, 2003.
3. Kenneth J. Klabunde (Ed), Nanoscale materials in Chemistry, Wiley- Interscience, New York, 2001.
4. T. Pradeep, Nano: The Essentials in understanding nanoscience and nanotechnology, Tata McGraw Hill, New Delhi, 2007.
5. H. Fujita (Ed.), Micromachines as tools in nanotechnology, Springer- Verlag, Berlin, 2003.
6. Bengt Nolting, Methods in modern biophysics, Springer-Verlarg, Berlin, First Indian Reprint, 2004. (Pages 102-146 for Unit II and 147 – 163 for UnitV)

7. H. Gleiter, Nanostructured Materials: Basic Concepts, Microstructure and Properties
8. W. Kain and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John-Wiley R Sons, NewYork.
9. T. Tangand P.Sheng(Eds), Nano Science and Technology Novel Structures and Phenomena,Taylor & Francis, New York, 2004.
10. A. Nabok, Organic and Inorganic Nanostructures, Artech House, Boston, 2005.
11. Edward A. Rietman, Molecular engineering of Nanosystems, Springer- Verlag, New York, 2001.
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M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV

SJCHE4C12: INSTRUMENTAL METHODS OF ANALYSIS

(4 Credits, 72h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To study the errors in Chemical analysis	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO2	To study the principle and working of various optical instruments	To develop skills in the proper handling of instruments	Z	C	9	Nil
CO3	To understand the working and application of various analytical instruments	To develop skills in the proper handling of instruments.	Z	F	8	Nil
CO4	To understand the principle of conventional analytical procedures	To develop the ability for applying the principles of chemistry.	A	F	10	Nil
CO5	To study the thermal and radiochemical methods.	To develop the ability for applying the principles of chemistry.	A	C	9	Nil
CO6	To understand the basic principle of Chromatography.	To be exposed to the different processes used in industries and their applications	U	C	9	Nil

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Errors in Chemical Analysis (9h)

Treatment of analytical data. Accuracy and precision. Absolute and relative errors. Classification and minimization of errors. Significant figures. Statistical treatment- mean and standard deviation, variance, confidence limits, student-t and f tests. Detection of gross errors, rejection of a result-Q test. Least square method, linear regression; covariance and correlation coefficient

Unit 2: Conventional Analytical Procedures (9h)

Gravimetry: solubility product and properties of precipitates-nucleation, growth and aging, co- precipitation and post precipitation, drying and ignition. Inorganic precipitating agents: NH3, H2S, H2SO4, (NH4)2MoO4 and NH4SCN. Organic precipitating agents: oxine, cupron, cupferron, 1-nitroso-l-naphthol, dithiocarbamates. Acid-Base and precipitation titrations: theory of neutralisation titrations, indicators for acid/base titrations, titration curves of strong acid, strong base, weak acid, weak base and polyprotic acids. Buffer solutions. Titrations in nonaqueous media. Different solvents and their selection for a titration. Indicators for non- aqueous titrations. Redox titrations: Permanganometry, dichcrometry, iodometry, cerimetry. Variation of potential during a redox titration, formal potential during a redox titration, Redox indicators. Precipitation titrations, adsorption indicators. Complexometric titrations: Types of EDTA titrations (direct, back, replacement, alkalimetric and exchange reactions), masking and demasking agents, selective demasking, metal ion indicators - murexide, eriochrome black T, Patton and Reeder's indicators, bromopyrogallol red, xylenol orange, variamine blue.

Unit 3: Electro Analytical Methods- I (9h)

Potentiometry: techniques based on potential measurements, direct potentiometric systems, different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, modern modifications, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. Polarography micro electrode and their specialities, potential and current variations at the micro electrode systems, conventional techniques for concentration determination, limitations of detection at lower concentrations, techniques of improving detection limit-rapid scan, ac, pulse, differential pulse square wave polarographic techniques. Applications of polarography.

Unit 4 Electro Analytical Methods II (9h)

Amperometry: biamperometry, amperometric titrations. Coulometry-primary and secondary coulometry, advantages of coulometric titrations, applications. Principle of chronopotentiometry. Anodic stripping voltammetry-different types of electrodes and improvements of lower detection limits. Voltammetric sensors. Organic polarography.

Unit 5 Optical Methods - I (9 h)

Fundamental laws of spectrophotometry, nephelometry and turbidometry and fluorimetry. UV- visible and IR spectrophotometry – instrumentation, single and double beam instruments, Spectrophotometric titrations. Atomic emission spectrometry – excitation sources (flame, AC and DC arc), spark, inductively coupled plasma, glue discharge, laser microprobes, flame structure, instrumentation, and qualitative and quantitative analysis. Atomic absorption spectrometry: sample atomization techniques, instrumentation, interferences, background correction, and analytical applications.

Unit 6 Optical Methods - II (9 h)

Theory, instrumentation and applications of: - Atomic fluorescence spectrometry, X-ray methods- X-ray absorption and X-ray diffraction, photoelectron spectroscopy, Auger, ESCA. SEM, TEM, and AFM

Unit 7: Thermal and Radiochemical Methods (9h)

Thermogravimetry (TG), Differential Thermal Analysis(DTA) and Differential Scanning Calorimetry(DSC) and their instrumentation. Thermometric Titrations. Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications. Principle and applications of isotope dilution methods.

Unit 8: Chromatography (9 h)

Chromatography-classification, column, paper and thin layer chromatography. HPLC-outline study of instrument modules. Ion – exchange chromatography-Theory. Important applications of chromatographic techniques. Gel Permeation Chromatography. Gas chromatography – basic instrumental set up-carriers, columns, detectors and comparative study of TCD, FID, ECD and NPD. Qualitative and quantitative studies using GC, Preparation of GC columns,

selection of stationary phases of GLC, Gas adsorption chromatography, applications, CHN analysis by GC.

References:

1. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.

2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry,

9th Edn ., Cengage Learning., 2014.

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8. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.

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Edition, Wiley-VCH, 2006.

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21.Yoshihiro Hamakawa, Thin-Film Solar Cells-Next Generation Photovoltaics and Its Applications, Springer Series in Photonics 13, 2008.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV

SJCHE4E04: PETROCHEMICALS AND COSMETICS (ELECTIVE)

(4 Credits, 72 hrs)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the basics of petroleum chemistry	To develop the ability for applying the principles of chemistry.	U	F	16	Nil
CO2	To study the preparation and purification of petrochemicals	To be exposed to the different processes used in industries and their applications.	A	P	20	Nil
CO3	To understand the classification and properties of petroleum products	To develop the ability for applying the principles of chemistry.	U	F	18	Nil
CO4	To study the preparation, composition and properties of perfumes & cosmetics	To be exposed to the different processes used in industries and their applications.	A	P	16	Nil

***R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create**

***F-factual, C-conceptual, P-practical/procedural**

Unit 1: Introduction to Petrochemistry (9h)

Introduction. Petroleum. Refining of crude oil. Fuels for internal combustion engines. Knocking, Octane number. Unleaded petrol. Diesel Engine and Cetane number. Cracking. Thermal, Catalytic. Mechanism of cracking process. Reforming Activation Gasoline. Petrochemicals.

Unit 2: Hydrocarbons from Petroleum (9h)

Introduction. Raw materials. Saturated hydrocarbons from natural gas. Uses of saturated hydrocarbons. Unsaturated hydrocarbons – Acetylene, Ethylene, Propylene, Butylenes. Aromatic hydrocarbons - Benzene. Toluene. Xylenes. Chemical processing of paraffin hydrocarbons. Chemical processing of ethylene hydrocarbons. Chemical processing of acetylene. Chemical processing of aromatic hydrocarbons.

Unit 3: Industrial Organic Synthesis (9h)

Introduction. The raw materials and basic processes. Chemical process used in industrial organic synthesis. Petrochemicals- Methanol. Important points. Ethanol. Important points. Rectified spirit from beer. Methylated spirit. Proof spirit. Preparation of the absolute alcohol from rectified spirit. Acetaldehyde. Acetic acid. Isopropanol. Ethylene glycol. Glycerine. Acetone. Phenol. Formaldehyde. Important points. Ethyl acetate. Important points.

Unit 4: Composition of Petroleum Crude (9h)

Composition of petroleum crude. Composition of the petroleum products. Isomeric compounds. Classification of petroleum crude. A survey of the world crude. Sulphur compounds in petroleum. Physical Properties and Test Methods. 1. Viscosity: Other methods for finding out viscosity. Viscosity of an oil blend. Use of the figure for finding out viscosity. Viscosities of hydrocarbons. 2. Density, 3. Surface and interfacial tensions. 4. Refractive Index. 5. Flash and fire points. 6. Cloud and pour points. 7. Aniline point. 8. Diesel index. 9. Cetane number. 10. Octane number and knock characteristics. 11. Distillation curves. (a) ASTM (American Society for Testing Materials) distillation curve. (b). Hempel or semi fractionating distillation curve.

Unit 5: Distillation of Crude Petroleum (9h)

Preparation of petroleum for processing. Destruction of petroleum emulsion. Electric desalting plants. Fundamentals of preliminary distillation. Methods of petroleum distillation. Distillation of crude petroleum. Treatment of the residual liquid processing of liquid fuels such as petroleum and petroleum products. Petroleum processing equipments. Storage tanks. Rectification columns. Cap tray or bubble tray columns. Heat exchange apparatus. Steam space heaters or boilers. Condensers. Pipe furnaces. Pipelines. Fitting Compressors and pumps.

Unit 6: Petroleum Products (9h)

Introduction. Classification of petroleum products. Liquefied hydrocarbons, gases and fuels. Fuel oils or boiler oils. Fuel for Jet engines and gas turbine engines. Lubricants, products of oil paraffine processing and other petroleum products. Lubricating and other oils. Paraffins, ceresins, petroleum. Miscellaneous petroleum products. Products of petrochemical and basic organic synthesis. Dye intermediates. Lacquers. Solvents. Thinners.

Unit 7: Purification of Petroleum Products (9h)

Absorptive and adsorptive purification. Sulphuric acid purification. Alkaline purification. Hydrorefining. Purification in a DC electric field. New methods of purification. De mercaptanisation. Stabilisation.

Unit 8: Perfumes and Cosmetics (9h)

Perfumes: Introduction. Esters. Alcohols. Ketones. Ionones. Nitromusks. Aldehydes. Diphenyl compounds. Production of natural perfumes. Flower perfume. Fruit flavours. Artificial flavours.

Cosmetics: Introduction. Toothpaste. Ingradients. Preparation. Recipe for toothpaste. Shampoos. Ingradients. Recipe. Hair dyeing. Materials used. Colour and Curl of Hair. Creams and Lotions. Skin Chemicals. Their ingradients. Preparation and recipe. Lipsticks. Ingradients. Preparation and recipe. Perfumes, Colognes and after shave preparation. Compounds with flowery and fruity odours used in perfumes with their structures. Compounds with unpleasant odours used to fix delicate odours in perfumes. Deodorants and Antiperspirants.

Cosmetics: Economics and Advertising.

References:

1. B. K. Sharma, Industrial Chemistry, Goel Publication, Goa.

2. N. K. Sinha, Petroleum Refining and petrochemicals,

3. John W. Hill, Chemistry for Changing times, Surjeet Publication

4. Uttam Ray Chaudhuri, "Fundamentals of Petroleum and Petrochemical Engineering",

Boca Raton London New York.

5. S ukumar Maiti, "Introduction to Petrochemicals" India Book House Pvt Ltd.

6. Gabriella Baki, Kenneth S. Alexander, "Introduction to Cosmetic Formulation and Technology", Wiley.

7. Tony Curtis, David Williams, "Introduction to Perfumery", Micelle Press; 2nd edition

M.SC. CHEMISTRY (CSS PATTERN) - SEMESTER IV

SJCHE4E05: INDUSTRIAL CATALYSIS

(4 CREDITS, 72 HRS)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To study the principles of catalysis	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO2	To understand the synthesis of different catalyst	To develop the ability for applying the principles of chemistry.	A	C	9	Nil
CO3	To study deactivation of Catalysts	To develop the ability for applying the principles of chemistry.	E	C	9	Nil
CO4	To understand the basic concepts in phase transfer catalysis	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO5	To study the industrial catalysis.	To be exposed to the different processes used in industries and their applications	A	C	9	Nil
CO6	To study the biocatalysis	To develop the ability for applying the principles of chemistry.	U	F	9	Nil

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Introduction to Adsorption process (9h)

Intermolecular interactions, physisorption. The forces of adsorption. Dispersion and repulsive forces. Classical electrostatic interactions. Adsorbate-adsorbate interactions, chemisorption, potential energy curves, thermodynamics of adsorption. Isothermal and adiabatic heats of adsorption. Variation of heats of adsorption with coverage. Adsorption isotherms, Langmuir, BET and Freundlich. Kinetics of chemisorptions. Activated and non- activated chemisorptions. Absolute rate theory. Electronic theories. Hysteresis and shapes of capillaries.

Unit 2: Kinetics and Catalysis (9h)

Adsorption and catalysis. Adsorption and reaction rate. Strength of adsorption bond and catalysis. Adsorption equilibrium and catalysis. Kinetics of heterogeneous catalysis: diffusion steps neglected. Unimolecular reactions. Bimolecular reactions. Langmuir- Hinshelwood and Eley-Rideal mechanism. Kinetics of heterogeneous catalysis: diffusion controlling. Mechanism of diffusion. Diffusion and reaction in pores. Selectivity and diffusion. Electronic factors in catalysis by metals, electronic factors in catalysis by semiconductors, geometric factors and catalysis.

References:

1. A. Clark, "Theory of adsorption and catalysis", Academic Press, 1970.

2. J.M. Thomas & W.J. Thomas, "Introduction to principles of heterogeneous catalysis",

Academic Press, New York, 1967.

3. R.H.P. Gasser, "An introduction to chemisorption and catalysis by metals", Oxford, 1985.

4. D.K Chakraborthy, "Adsorption and catalysis by solids", Wiley Eastern Ltd. 1990.

Unit 3: Catalyst - Preparative Methods (9h)

Surface area and porosity measurement. Measurement of acidity of surfaces. Support materials. Preparation and structure of supports. Surface properties. Preparation of catalysts. Introduction of precursor compound. Pre-activation treatment. Activation process. General methods of synthesis of zeolites. Mechanism of nuclear formation and crystal growth. Structures of some selected zeolites. Zeolites A, X and Y. Pentasils. ZSM-5. ZSM-11. Shape selective catalysis by zeolites.

Unit 4: Deactivation of Catalysts (9h)

Deactivation of catalysts. Classification of catalyst deactivation processes. Poisoning of catalysts. Coke formation on catalysts. Metal deposition on catalysts. Sintering of catalysts. Regeneration of deactivated catalysts. Feasibility of regeneration. Description of coke deposit and kinetics of regeneration.

References:

1. J.R. Anderson and M. Boudart (Eds), "Catalysis, Science and Technology", Vol 6, Springer- Verlag, Berlin Heildberg, 1984.

2. R.B. Anderson, "Experimental methods in catalysis research", Vol I, II, Academic press, NY, 1981.

3. R. Szostak, "Molecular sieves: principles of synthesis and identification", Van Nostrand, NY, 1989.

4. R. Hughes, "Deactivation of catalysts", Academic press, London, 1984.

Unit 5: Phase Transfer Catalysis (9h)

Basic concepts in phase transfer catalysis. Phase transfer catalyzed reactions. Basic steps of phase transfer catalysis. Effect of reaction variables on transfer and intrinsic rates. Outline of compounds used as phase transfer catalysts. Use of quaternary salts. Macrocyclic and macrobicyclic ligands. PEG's and related compounds. Use of dual phase transfer catalyst or co-catalyst in phase transfer systems. Separation and recovery of phase transfer catalysts. Insoluble phase transfer catalysts.

Unit 6: Biocatalysis (9h)

Enzymes. An introduction to enzymes. Enzymes as proteins. Classification and nomenclature of enzymes. Structure of enzymes. How enzymes work. Effect on reaction rate. Thermodynamic definitions. Catalytic power and specificity of enzymes. Optimization of weak interactions between enzyme and substrate in the transition state. Binding energy, reaction specificity and catalysis. Specific catalytic groups contributing to catalysis. Immobilized biocatalysts. Definition and classification of immobilized biocatalysts. Immobilization of coenzymes.

References:

1. C.M. Starks, C.L. Liotta and M. Halpern, "Phase Transfer Catalysis – Fundamentals, Applications and Industrial Perspectives", Chapman & Hall, New York, 1994.

2. A.L. Lehninger, "Principles of Biochemistry", Worth Publishers, USA, 1987.

Unit 7: Industrial Catalysis-1 (9h)

Oil based chemistry. Catalytic reforming. Catalytic cracking. Paraffin cracking. Naphthenic cracking. Aromatic hydrocarbon cracking. Isomerization. Hydrotreatment. Hydrodesulphurization. Hydrocracking. Steam cracking. Hydrocarbons from synthesis gas. Fisher-Tropsch process. Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

UNIT 8: Industrial Catalysis-II (9h)

Hydroformylation of olefins. Carbonylation of organic substrates. Conversion of methanol to acetic acid. Synthesis of vinyl acetate and acetic anhydride. Palladium catalyzed oxidation of ethylene. Acrylonitrile synthesis. Zeigler-Natta catalysts for olefin polymerization. Propene polymerization with silica supported metallocene/MAO catalysts.

References:

1. G. Ertl, H. Knozinger and J. Weitkamp, "Handbook of Heterogeneous Catalysis" Vol 1- 5, Wiley-VCH, Weinheim, 1997.

2. R.J. Farrauto and C.H. Bartholomew, "Fundamentals of Industrial Catalytic Processes",

Blackie Academic and Professional – Chapman and Hall, 1997.

3. R. Pearce and W.R. Patterson, "Catalysis and chemical processes", Academic press, Leonard Hill, London, 1981.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV

SJCHE4E06: NATURAL PRODUCTS & POLYMER CHEMISTRY (ELECTIVE)

(4 Credits, 72 hrs)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the structure and properties of natural products- Terpinoids, steroids, and alkaloids	To develop the ability for applying the principles of chemistry.	U	F	15	Nil
CO2	To understand the structure and properties anthocyanins, dyes, pigments and supramolecules	To develop the ability for applying the principles of chemistry.	U	P	15	Nil
CO3	To understand the mechanism, characterization and stereochemistry of polymers	To develop the ability for applying the principles of chemistry.	U	F	24	Nil
CO4	To study synthesis, structure and applications of different types of polymers	To be exposed to the different processes used in industries and their applications.	A	F	18	Nil

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

UNIT 1: Basic aspects of Natural Products (9 h)

Classification of Natural Products: Classification of Natural products based on chemical structure, physiological activity, taxonomy and Biogenesis. Carbohydrates. Terpenoids. Carotenoids. Alkaloids. Steroids. Anthocyanins etc. Methods of isolation of each class of compound. Essential Oils: Isolation and study of important constituents of lemon grass oil, citronella oil, cinnamon oil, palmarosa oil, turpentine oil, clove oil, sandalwood oil, Essential oils of turmeric and ginger. Oleoresins of pepper, chilly, ginger and turmeric. Aromatherapy.

UNIT 2: Terpenoids and Steroids (9 h)

Terpenoids: classification, structure elucidation and synthesis of abietic acid.
Steroids: Classification, structure of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone. Classification, structure and synthesis of prostaglandins, biosynthesis of fatty acids, prostaglandins, terpenoids and steroids. Structural elucidation of Cholesterol, Ergosterol, Oesterone, Androsterone, Testosterone, Progestrone, Cortisone and Corticosterone.

UNIT 3: Alkaloids and Anthocyanins (9 h)

Alkaloids. Classification of alkaloids, structural elucidation based on degradative reactions (quinine and atropine). Biosynthesis of quinine and papaverine.
Anthocyanins: Introduction, General Nature and Structure of Anthocyanidins. Flavone, Flavonol, Isoflavone and Chalcone

UNIT 4: Dyes, Pigments and Supramolecules (9 h)

Brief introduction to dyes and pigments (natural and synthetic): β-carotene, indigo, cyclic tetrapyrroles (porphyrins, chlorins, chlorophyll, heme). Study of phthalocyanines, squarenes, and cyanine dyes. Introduction to Supramolecular chemistry and Molecular Recognition

References:

1. M. B. Smith, Organic Synthesis, 3/e, Academic Press, 2011.
2. F. A. Carey and R. J. Sundberg: Advanced Organic Chemistry (part B), 3rd ed., Plenum Press.
3. T.W. G. Solomons: Fundamentals of Organic Chemistry, 5th ed., John Wiley
4. H. O. House: Modern Synthetic Reactions, W. A. Benjamin

5. W. Carruthers: Some Modern Methods of Organic Synthesis, 4/e, CambridgeUniversity Press.
6. I. L. Finar: Organic Chemistry Volumes 1 (6th ed.) and 2 (5th ed.), Pearson.
7. J. Clayden, N. Green, S. Warren and P. Wothers: Organic Chemistry, 2/e, OxfordUniversity Press
8. N. R. Krishnaswamy: Chemistry of Natural Products; A Unified Approach, Universities Press
9. R. J. Simmonds: Chemistry of Biomolecules: An Introduction, RSC
10. R. O. C. Norman: Principles of Organic Synthesis, 3nd ed., CRC Press, 1998.
11. J. M. Lehn, Supramolecular Chemistry

UNIT 5: Polymerization Processes (9 h)

Polymerization processes. Free radical addition polymerization. Kinetics and mechanism. Chain transfer. Mayo-walling equation of the steady state. Molecular weight distribution and molecular weight control. Radical Atom Transfer and Fragmentation – Addition mechanism. Free radical living polymers. Cationic and anionic polymerization. Kinetics and mechanism, Polymerization without termination. Living polymers. Step Growth polymerization. Kinetics and mechanism. Molecular weight distribution. Linear Vs cyclic polymerization, other modes of polymerization. Group Transfer, metathesis and ring opening polymerization. Copolymerization. The copolymerization equation, Q-e scheme, Gelation and Crosslinking. Copolymer composition drift Polymerization techniques. Bulk Solution, melt, suspension, emulsion and dispersion techniques

UNIT 6: Characterization and Stereochemistry of Polymers (9 h)

Polymer Stereochemistry. Organizational features of polymer chains. Configuration and conformation, Tacticity, Repeating units with more than one asymmetric center. Chiral polymers– main chain and side chain. Stereoregular polymers. Manipulation of polymerization processes. Zeigler-Natta and Kaminsky routes. Coordination polymerization. Metallocene and Metal oxide catalysts. Polymer Characterization. Molecular weights. Concept of average molecular weights, Molecular weight distribution. Methods for determining molecular weights. Static and dynamic methods, Light scattering and GPC. Crystalline and amorphous states. Glassy and Rubbery States. Glass transition and crystalline melting. Spherullites and Lammellac. Degree of Crystallinity, X-ray diffraction

UNIT 7: Polymer Solutions, Industrial polymers and Copolymers (9 h)

Polymer Solutions. Treatment of dilute solution data. Thermodynamics. Flory-Huggins equation. Chain dimension-chain stiffness – End-to-end distance. Conformation-random coil, Solvation and Swelling. Flory-Reiner equation. Determination of degree of crosslinking and molecular weight between crosslinks. Industrial polymers. Synthesis, Structure and applications. Polyethylene, polypropylene, polystyrene. Homo and Copolymers. Diene rubbers. Vinyl and acrylic polymers. PVC, PVA, PAN, PMMA and related polymers. Copolymers. EVA polymers. Flourine containing polymers. Polyacetals. Reaction polymers. Polyamides, polyesters. Epoxides, polyurethanes, polycarbonates, phenolics, PEEK, Silicone polymers.

UNIT 8: Speciality Polymers (9 h)

Reactions of polymers. Polymers as aids in Organic Synthesis. Polymeric Reagents, Catalysts, Substrates, Liquid Crystalline polymers. Main chain and side chain liquid crystalline polymers. Phase morphology. Conducting polymers. Polymers with high bandwidth. Polyanilines, polypyrrols, polythiophines, poly (vinylene phenylene). Photoresponsive and photorefractive polymers. Polymers in optical lithography. Polymer photoresists. Electrical properties of Polymers, Polymers with NLO properties, second and third harmonic generation, and wave guide devises.

References:

1. F.W. Billmayer. Textbook of Polymer Science. 3rd Edn, Wiley. N.Y. 1991.

2. G. Odiyan, Principles of Polymerisation, 4/e, Wiley, 2004.

3. V.R. Gowriker and Others, Polymer Science, Wiley Eastern Ltd.

4. J.M.G Cowie. Polymers: Physics and Chemistry of Modern Materials. Blackie. London, 1992.

5. R.J.Young, Principles of Polymer Science, 3rd Edn. , Chapman and Hall. N.Y. 1991.

6. P.J. Flory. A Text Book of Polymer Science. Cornell University Press. Ithacka, 1953.

7. F. Ullrich, Industrial Polymers, Kluwer, N.Y. 1993.

8. H.G.Elias, Macromolecules, Vol. I & II, Academic, N.Y. 1991.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV

SJCHE4E07: MATERIAL SCIENCE (ELECTIVE)

(4Credits, 72 hrs)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand classification and properties of ceramic, nano and composite materials	To develop the ability for applying the principles of chemistry.	U	F	18	Nil
CO2	To study the mechanical, electrical and magnetic properties of polymers	To be exposed to the different processes used in industries and their applications.	A	F	24	Nil
CO3	To appreciate the importance of nanotechnology	To be exposed to the different processes used in industries and their applications.	A	F	18	Nil
CO4	To understand the importance of fracture mechanics	To be exposed to the different processes used in industries and their applications.	U	F	12	Nil

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Introduction to Material Science (9h)

Introduction. Classification of materials. Functional classification. Classification based on structure. Environmental and other effects. Material design and selection;
Mechanical properties – significance and terminology, the tensile test, true stress and true strain, bend test, hardness of materials.

Unit 2: Ceramic Materials (9h)

Definition of ceramics. Traditional and new ceramics. Structure of ceramics. Atomic interactions and types of bonds. Phase equilibria in ceramic systems, one component and multi component systems. Use of phase diagrams in predicting material behavior. Electrical, magnetic, and optical properties of ceramic materials.

Unit 3: Nanomaterials and Nanotechnology (9h)

Nanomaterials. Nanostructures. Self-assembly. Nanoparticles- methods of synthesis, sol-gel process, hydrolysis of salts and alkoxides, precipitation, condensation reactions, electrokinetic potential and peptization reactions. Gelatin network- xerogels, aerogels, drying of gels. Chemical modifications of nanosurfaces. Applications of sol-gel process, sol-gel coating, porous solids, catalysts, dispersions and powders

Unit 4: Materials for Special Purposes – I (9h)

Production of ultra-pure materials - zone refining, vacuum distillation and electro refining. Ferroelectric and piezoelectric materials - general properties. Classification of ferroelectric materials. Theory of ferroelectricity, ferroelectric domains, applications. Piezoelectric materials and applications. Metallic glasses - preparation, properties and applications.

Unit 5: Materials for Special Purposes – II (9h)

Magnetic materials, ferri and ferro magnetism. Metallic magnets, soft, hard & superconducting magnets. Ceramic magnets, low conducting and superconducting magnets. Superconducting materials - metallic and ceramic superconducting materials, theories of superconductivity. Meissner effect. High temperature superconductors - structure and applications.

Unit 6: Some Special Polymers (9h)

Functional polymers - photoconductive, electroconductive, piezoelectric and light sensitive polymers. Industrial polymers - production, properties, & compounding of industrial polymers. Commodity plastics such as PP, PE, PVC, & PS. Engineering plastics such as polyacetyl, polyamide (nylon 6 and nylon 66), polyacrylate, polycarbonate, polyester (PET, PBT), polyether ketones. Thermosetting plastics such as PF, UF & MF.

Unit 7: Composite Materials (9h)

Definition and classification of composites, fibres and matrices. Composites with metallic matrices – processing, solid and liquid state processing, deposition. Ceramic matrix composite materials – processing, mixing & Pressing, liquid state processing, sol-gel processing & vapor deposition technique. Interfaces in composites - mechanical & microstructural characteristics. Applications of composites.

Unit 8: Fracture Mechanics (9h)

Importance of fracture mechanics. Micro structural features of fracture in metals, ceramics, glasses & composites. Weibull statistics for failure, strength analysis. Fatigue, application of fatigue testing - creep, stress rupture & stress behavior, evaluation of creep behavior.

References:

1. W.D. Eingery, H.K. Dowen and R.D. Uhlman, Introduction to Ceramics, John Wiley.

2. A.G. Guy, Essentials of Material Science, McGraw Hill.

3. M.J. Starfield and Shrager, Introductory Material Science, McGraw Hill.

4. S.K. Hajra Choudhary, Material Science and Engineering, Indian Book Dist. Co., Calcutta.

5. M.W. Barsoum, Fundamentals of Ceramics, McGraw Hill, 1997.

6. M. Tinkham, Introduction to Superconductivity, McGraw Hill, 1975.

7. A.V. Narlikar and S.N.Edbote, Superconductivity and Superconducting Materials, South Asian Publishers, New Delhi, 1983.

8. S.V. Subramanyan and E.S. Rajagopal, High Temperature Superconductors, Wiley Eastern Ltd., 1988.

9. Azaroff and Brophy, Electronic Processes in Materials, McGraw Hill, 1985.

10. C.M. Srivastava and C. Srinivasan, Science of Engineering Materials, Wiley Eastern Ltd., 1987. R.J. Young, Introduction to Polymer Science, John Wiley and Sons.

11. V.R. Gowriker and Others, Polymer Science, Wiley Eastern Ltd.

12. H. Ulrich, Introduction to Industrial Polymers, Hansen Publishers, 1982.

13. F.R. Jones, Handbook of Polymer Fibre Composites, Longman Scientific and Tech.

14.K.K. Chowla, Composite Materials, Springer-Verlag, NY, 1987.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV CHE4E08 – ORGANOMETALLIC CHEMISTRY (ELECTIVE)

(4 credits, 72h)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the stability of metal carbonyls.	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO2	To understand the structure and synthesis of organometallic pi-complexes.	To develop the ability for applying the principles of chemistry.	U	C	9	Nil
CO3	To understand the applications of organometallic compounds.	To be exposed to the different processes used in industries and their applications	A	C	9	Nil
CO4	To analyse bonding pattern and stability of organometallic compounds.	To develop the ability for applying the principles of chemistry.	Z	C	9	Nil
CO5	To understand the reactivity and reactions given by organometallic compounds.	To develop the ability for applying the principles of chemistry.	U	C	9	Nil
CO6	To understand the stability of organometallic compounds using 18-electron rule.	To develop the ability for applying the principles of chemistry.	U	C	9	Nil

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

UNIT I (9h)

Organometallic compounds. Classification and nomenclature. The 16 and 18 electron rules. Electron counting-covalent and ionic models. Main group organometallics-alkyl and aryl, groups 1, 2, 12, 13, 14 and 15 synthesis, structure and applications. Transition metal to carbon multiple bond-the metal carbenes and carbynes. Transition metal complexes with chain π ligands – synthesis, structure, bonding and reactions of complexes of ethylene, allyl, butadiene and acetylene.

UNIT II (9h)

Metal carbonyls- Bonding modes of CO. IR spectroscopy as a tool to study bonding and structure of metal carbonyls. Synthesis of Metal carbonyls, Direct and reductive Carbonylation. Reactions of Metal carbonyls-Activation of metal carbonyls, Disproportion, Nucleophilic addition, electrophilic addition to the carbonyl oxygen, Carbonyl cation, anions and hydrides. Collmann's reagent, Migratory insertion of carbonyls. Oxidative decarbonylation. Photochemical substitution. Microwave assisted substitution.

UNIT III (9h)

General aspects of synthesis. Structure, reactivity and applications of main group organometallic compounds. Metal complexes of NO, H2, CS, RNC and Phosphines. Metal-carbon multiple bonds- Metal carbenes and carbynes, bridging carbenes and carbynes, N-heterocyclic carbons, multiple bonds to hetero atoms.

UNIT IV (9h)

Organometallic π complexes – synthesis, structure, bonding (molecular orbital treatment) and reactions of C_5H_5, C_6H_6, C_7H_7 and $C_8H_8^{2-}$. Polyalkyls, polyhydrides and f-block organometallic complexes, Fluxional organometallics.

UNIT V (9h)

Applications of organometallic compounds in organic synthesis and homogeneous catalysis, Complex formation and activation of H2, N2, O2, NO by transition metals. Catalytic steps, Oxidative addition, reductive elimination and insertion reactions. Hydrozirconation of alkenes and alkynes. Homogeneous catalysis. Hydrogenation, isomerization of alkenes, alkyne, cycloadditions, Zeigler-Natta catalysis, hydroformylation of alkenes, Monsanto acetic acid process and Wacker process. Metal complexes in enantioselective synthesis

UNIT VI (9h)

Organometallic reactions. SN2 Reactions, Radical Mechanisms, Ionic Mechanisms, σ-Bond Metathesis, Oxidative Coupling and Reductive decoupling. Reactions involving CO, Insertions Involving Alkenes, Other Insertions, α, β, γ and δ Elimination, Deinsertion and Nucleophilic and electrophilic attack on coordinated ligand.

UNIT VII (9h)

Applications of organometallic reaction. Homogeneous catalysis. General features of catalysis. Types of catalyst. Catalytic steps. Water-gas shift reaction. Fisher-Tropsch reaction. Hydrosilation of alkenes. Hydrocyanation of alkenes.

UNIT VIII (9h)

Organometallic Polymers. 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 oly(ferrocenylsilane)s and related polymers. Applications of rigid-rod polyynes, polygermanes and polystannanes. Polymers prepared by ring opening polymerization. Organometallic dendrimers.

References:

1. B. D. Gupta, A .J. Elias, Basic Organometallic Chemistry - Concepts, Synthesis and Applications, Second edition, University Press, 2013.

2. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, Fourth edn. 2005, Wiley Interscience.

3. J. E. Huheey, Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, Pearson education, 1993.

4. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry. 5th edition, John and Wiley, 1999.

5. R.S. Drago. Physical Methods in Inorganic Chemistry, 2nd edition, affiliated east west press, 1993.

6. P. Powell, Principles of Organomettalic Chemistry, 2nd edition, Chapman and Hall, London, 1998.

7. S. F. A. Kettle, Concise co-ordination chemistry, Nelson, 1969.

8. S. F. A. Kettle, Physical Inorganic Chemistry-A Co-ordination chemistry Approach, Spectrum academy publishers, 1996.

9. Purcell and Kotz, Inorganic Chemistry. 10. D. J. Shriver, P. W. Atkins, Inorganic Chemistry, 5th edition, Oxford university press, 2010.

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV

SJCHE4E09: MEDICINAL & COMBINATORIAL CHEMISTRY (ELECTIVE)

(4 Credits, 72 hrs)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To understand the classification and pharmacological activity of drugs	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO2	To study SAR, QSAR of drugs & drug design, immunoassays and nanomedical applications	To be exposed to the different processes used in industries and their applications.	A	P	18	Nil
CO3	To understand the medical applications of essential oils	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO4	To understand the structure, synthesis and properties of terpenoids and steroids	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO5	To understand the basic principles and methods of combinatorial synthesis	To develop the ability for applying the principles of chemistry.	U	F	9	Nil
CO6	To apply combinatorial chemistry in drug design	To be exposed to the different processes used in industries and their applications.	A	P	18	Nil

***R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create**

***F-factual, C-conceptual, P-practical/procedural**

UNIT 1: Medicinal Chemistry I (9 h)

Introduction, different classes of drugs, drug action, prodrugs, physico chemical properties of drugs and their pharmacologic activity, pharmacokinetics (ADME), pharmacodynamics, pharmacophore, lead discovery- lead optimization- drugability- Lipinski rule of five-drug design and relationship of functional groups to pharmacologicalactivity, natural products as lead structures in drug discovery- pharmacophore, discovery of lead compounds from natural hormones & neurotransmitters, Principles of design of agonists (eg.salbutamol), antagonists (eg. cimetidine), & enzyme inhibitors (captopril), drug discovery without lead- serendipity- (eg: penicillin), drug patents & clinical trials.

UNIT 2: Medicinal Chemistry II (12 h)

Structure Activity Relationships (SAR) in drug design: Qualitative versus quantitative approachesadvantages and disadvantages. Random screening, Non-random screening, drug metabolism studies, clinical observations, rational approaches to lead discovery. Homologation, chain branching, ring-chain transformations, bioisosterism. QSAR: Electronic effects: Hammett equation, lipophilicity effects. Hansch equation, stericeffects. Taft equation. Experimental and theoretical approaches for the determination of physico-chemical parameters, parameter inter-dependence; case studies. Regression analysis, extrapolation versus interpolation, linearity versus non-linearity. Descriptor calculation. The importance of biological data in the correct form; 2D QSAR; 3D-QSAR, rational approach to drug design, general methods of drug synthesis.

UNIT 3: Immunoassays (6 h)

Immunoassays: General principles, antigen -antibody interactions, Hapten inhibition test, immunodiffusion, immunoelectrophoresis, ELISA, ELOSA, Fluorescence immunoassay and Radio immunoassay. Biosensors and chemosensors

UNIT 4: Nanomedical Applications (9 h)

Drug delivery & drug delivery systems, nanoparticle in drug delivery- targeting ligands applications of nanoparticle in drug delivery, cancer treatment, nanoparticle, nanonephrology, nanosystems in inflammation, targeting macrophages to control inflammation, tissue regeneration, growth and repair, drug delivery technology significance, impact of drug discovery and development.

UNIT 5: Combinatorial Chemistry (9 h)

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, requirements-resins, Linkers. Reactants for solid phase synthesis. Methods of Parallel synthesis: Haughton`s tea bag procedure. Automated parallel synthesis. Methods in mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis. Structure determination of active compounds- Deconvolution. Methods in deconvolution recursive deconvolution, tagging use of decoded sheets. Planning and designing of combinatorial synthesis. Spider like scaffolds, drug molecules. Limitations of combinatorial chemistry.

UNIT 6: Combinatorial Synthesis in Medicinal Chemistry (9 h)

Combinatorial chemistry in drug discovery-Compound mixtures versus single compounds -Solid phase synthesis versus synthesis in solution -Combinatorial synthesis of Biopolymers -Linear, modular synthesis of biopolymers -Solid-phase synthesis of polypeptides, library synthesis planning -Synthesis strategies-Classical multi-component reactions (MCR's) -Sequential multi-component reactions (SMCR's) -Diversity-oriented synthesis (DOS) -Collective synthesis of natural products -Fragment-based lead discovery -Dynamic Combinatorial Synthesis; -Target-guided synthesis (TGS)

UNIT 7: Basic aspects of Natural Products (9 h)

Pharmacognosy – definition and scope in allopathic and ayurvedic medicine- Classification of Natural products based on chemical structure, physiological activity. Essential Oils: Isolation and study of important constituents of lemon grass oil, citronella oil, cinnamon oil, palmarosa oil, turpentine oil, clove oil, sandalwood oil, Essential oils of turmeric and ginger. Oleoresins of pepper, chilly, ginger and turmeric. Aromatherapy.

UNIT 8: Terpenoids and Steroids (9 h)

Terpenoids: classification, structure elucidation and synthesis of abietic acid. Steroids: Classification, structure of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone. Classification, structure and synthesis of prostaglandins, biosynthesis of fatty acids, prostaglandins, terpenoids and steroids. Structural elucidation of Cholesterol, Ergosterol, Oesterone, Androsterone, Testosterone, Progestrone, Cortisone and Corticosterone.

References:

1. Lemke, Williams, Roche and Zito, Principles of Medicinal Chemistry, 7/e, Wolters Kluwer,2012.
2. G.Thomas, Fundamentals of Medicinal Chemistry, Wiley.
3. G.Gringauz, Introduction to Medical Chemistry, Wiley-VCH, 1997.
4. Harkishan Singh and V.K.Kapoor, Medicinal and Pharmaceutical Chemistry, Vallabh Prakashan, 2008.
5. Nanotechnology: Importance and Application by M.H. Fulekar, IK International, 2010.
6. Nanotechnology in Biology and Medicine: Methods, Devices and Application by Tuan Vo-Dinh .CRC press, 2007.
7. Nanosystem characterization tools in the life sciences by Challa Kumar. Wiley-VCH, 2006.
8. Introduction to Nanoscience by Gabor L. Hornyak, Joydeep Dutta, Harry F. Tibbals, Anil K. Rao. CRC Press, 2008.
9. Cancer Nanotechnology, eds. H. S. Nalwa and Thomas Webster, American Scientific Publishers, 2007.
10. Introduction to Nanotechnology, Charles P. Poole, Jr., Frank J. Owens; John Wiley & Sons, 2003
11. W.Bannwarth and B.Hinzen, Combinatorial Chemistry-From Theory to Application, 2nd Edition, Wiley-VCH, 2006.
12. A.W.Czarnik and S.H.DeWitt, A Practical Guide to Combinatorial Chemistry, 1st Edition, American Chemical Society, 1997.
13. N. K. Terret: Combinatorial Chemistry, Oxford University Press, 1998.

14. Natural Products : Chemistry and Biological Significance, J. Mann, R.S. Davidson, J. B.

Hobbs, D. V. Banthrope and J. B Harborne, Longman, Essex. Organic Chemistry, Vo. 2. I. L. Finar, ELBS.

15. Chemistry, Biological and Pharmacological Properties of Medicinal plants from the Americas, Ed. Kurt Hostettmann, M. P. Gupta and A. marston, Harwood Academicpublishers.

16. New Trends in Natural Product chemistry, Atta-ur-Rahman and M. I. Choudhary, Harwood Academic Publishers.

M.Sc. CHEMISTRY – SEMESTER III & IV

CHE3L07 & CHE4L10 – INORGANIC CHEMISTRY PRACTICALS– III & IV

(3 Credits)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To introduce various food colours.	To develop skills in the proper handling of instruments and chemicals	R	P	Nil	9
CO2	To determine the purity of organic compounds by chromatographic methods.	. To develop skills in the proper handling of instruments and chemicals	A	P	Nil	9
CO3	To understand common methods of extraction of natural products.	. To develop skills in the proper handling of instruments and chemicals	U	P	Nil	10
CO4	To analyse organic compounds by quantitative methods.	To develop skills in the proper handling of instruments and chemicals	Z	P	Nil	10
CO5	To apply the principles of colourimetry to organic compounds.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	5

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Estimation of ions in mixture

Estimation involving quantitative separation of suitable binary mixtures of ions in solution (Cu^{2+}, Ni^{2+}, Zn^{2+}, Fe^{3+}, Ca^{2+}, Mg^{2+}, Ba^{2+} and $Cr_2O_7^{2-}$) by volumetric colorimetric or gravimetric methods only one of the components to be estimated.

Unit 2: Colorimetric Estimations

Colorimetric estimations of Ni, Cu, Fe and Mo, after separation from other ions in solution by solvent extraction. (Minimum two expts.)

Unit 3: Ion Exchange Methods

Ion-exchange separation and estimation of binary mixtures (Co^{2+} & Ni^{2+}, Zn^{2+} & Mg^{2+}. Hardness of water).

Unit 4: Preparation of Inorganic Complexes. (5 Nos)

References:

1.Vogel's Text Book of Qualitative InorganicAnalysis.

2.I.M. Kolthoff and E.A. Sanderson, Quantitative ChemicalAnalysis.

3.D.A. Adams and J.B. Rayner, Advanced Practical InorganicChemistry.

4.W.G.Palmer, Experimental InorganicChemistry.

5.G. Brauer, Hand book of Preparative Inorganic Chemistry.

M.Sc. CHEMISTRY – SEMESTER III & IV

CHE3L08 & CHE4L11 – ORGANIC CHEMISTRY PRACTICALS– III & IV (3 Credits)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To introduce various food colours.	To develop skills in the proper handling of instruments and chemicals	R	P	Nil	9
CO2	To determine the purity of organic compounds by chromatographic methods.	. To develop skills in the proper handling of instruments and chemicals	A	P	Nil	9
CO3	To understand common methods of extraction of natural products.	. To develop skills in the proper handling of instruments and chemicals	U	P	Nil	10
CO4	To analyse organic compounds by quantitative methods.	To develop skills in the proper handling of instruments and chemicals	Z	P	Nil	10
CO5	To apply the principles of colourimetry to organic compounds.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	5

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

Unit 1: Quantitative Organic Analysis

Estimation of equivalent weight of acids by Silver Salt method, Estimation of nitrogen by Kjeldahl method, Determination of Acid value, iodine value and saponification value of oils and fats (at least one each), estimation of reducing sugars, estimation of amino group, phenolic group and esters. Colourimetric estimations: Vitamins (Ascorbic acid), Drugs – sulpha drug (Sulpha diazine, sulphaguanidine), Antibiotics – Pencillin, Stroptomycin.

References:

1.B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, ELBS/Longman, 1989.

2.Beebet, Pharmacuetical Analysis.

Unit 2: Extractions

Extraction of Natural products and purification by column chromatography and TLC – Caffeine from Tea waste, Chlorophyll, Steroids, Flavonoid (Soxhlet extraction), citral from lemon grass (steam distillation). Casein from milk.

Unit 3: Chromatograhy

Practical application of PC and TLC, preparation of TLC plates, activation, identification of the following classes of compounds using one- and two-dimensional techniques. Identification by using spray reagents and co-chromatography by authentic samples and also from Rf values.

Food additives and Dyes, Artificial sweeteners: Saccharine, cyclamates, Dulcin. Flavour adulterants – piperonal, benzyl acetate, ethyl acetate antioxidants: Butylated hydroxytoluene (BHT) Butylated hydroxy anisole (BHA), Hydroquinone.

Food colours: Permitted – Amaranth, Erythrosine, Tatrazine, susnet yellow, Fast green, Brilliant Blue, Nonpermitted colours: Auramine, Congo red, Malachite green, Metanil yellow, Orange II, Sudan II, Congo red. Amino acids (Protein hydrolysates), Sugars, Terpinoids, Alkaloids, Flavonoids, Steroids.

Pesticides and herbicides: Oragonochlorine pesticides organo phosphates and carbamate pesticides, Herbicides.

Plant growth stimulants: Indole acetic acid.

References:

1.B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, 5/e, Pearson, 1989.

2. Beebet, PharmacueticalAnalysis

3. E. Hoftmann, Chromatography, non Nostrand Reinhold Company, New York, 1975.

4. J. Sherma and G. Zwig, TLC and LC analysis of pesticides of international importance, Vol. VI & VII, AcademicPress.

5. H. Wagner, S. Bladt, E.M. Zgainsti – Tram, Th. A. Scott., Plant Drug Analysis, Springer-Verlag, Tokyo,1984.

6.Vishnoi, Practical Organic Chemistry.

M.Sc. CHEMISTRY – SEMESTER III & IV

CHE3L09 & CHE4L12 – PHYSICAL CHEMISTRY PRACTICALS– III & IV
(3 Credits)

	Course Outcome	POs/ PSOs	CL	KC	Class Sessions (appr.)	Lab (Hrs)
CO1	To determine specific reaction rate.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	9
CO2	To determine phase diagram of a ternary liquid system.	. To develop skills in the proper handling of instruments and chemicals	A	P	Nil	9
CO3	. To determine surface area of adsorbent.	. To develop skills in the proper handling of instruments and chemicals	A	P	Nil	10
CO4	To determine molecular mass of a solute using depression in freezing point of a liquid solvent.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	10
CO5	To apply HF/6-31G level of theory to determine various physical constants.	To develop skills in the proper handling of instruments and chemicals	A	P	Nil	5

*R-remember, U-understand, A-apply, Z-analyze, E-evaluate, C-create
*F-factual, C-conceptual, P-practical/procedural

SECTION A

Unit 1: Chemical Kinetics (4 experiments)

1.Determination of specific reaction rate of acid hydrolysis of an ester (methyl acetate or ethyl acetate) and concentration of the given acids.

2.Determination of Arrhenius parameters of acid hydrolysis of an ester.

3.Determination of specific reaction rate of saponification of ethyl acetate.

4.Iodination of acetone in acid medium – Determination of order of reaction with respect of iodine and acetone.

Unit 2: Adsorption (3 experiments)

1.Verification of Langmuir adsorption isotherm– charcoal-aceticacid system. Determination of the concentration of a given acetic acid solution using the isotherm

2.Verification of Langmuir adsorption isothem– charcoal-oxalic acid system. Determination of the concentration of a given acetic acid solution using the isothem.

3. Determination of surface area of adsorbent.

Unit 3: Phase Equilibria (2 experiments)

1.(a)Determination of phase diagram of a ternary liquid system(e.g., chloroform– acetic acid – water, Benzene – acetic acid –water)

(b) Determination of the composition of a binary liquid mixture (e.g., chloroform-acetic acid, benzene-acetic acid)

2.(a) Determination of mutual miscibility curve of a binary liquid system (e.g., phenol – water) and critical solution temperature (CST).

(b)Effect of impurities (e.g, NaCl, KCl, succinic acid, salicylic acid) on the CST of water-phenol system

(c)Effect of a given impurity (e.g., KCl) on the CST of water–phenol system and determination of the concentration of the given solution of ---------

Unit 4: Cryoscopy – Beckman Thermometer Method (3 experiments)

1.Determination of cyroscopic constant of a liquid (water, benzene)

2.Determination of molecular mass of a solute (urea, glucose, cane sugar, mannitol) by studying the depression in freezing point of a liquid solvent (water, benzene)

3.Determination of Van't Hoff factor and percentage of dissociation of NaCl.

4.Study of the reaction 2Kl + Hgl2 →.K2Hgl4 and determination of the concentration of the given Kl solution.

Unit 5: Polarimetry (3 experiments)

1.Determination of specific and molar optical rotations of glucose, fructose and sucrose.

2.Determination of specific rate of inversion of cane sugar in presence of HCl.

3.Determination of concentration of HCl

Unit 6: Spectrophotometry (3 experiments)

1.Determination of equilibrium constants of acid –base indicators.

2.Simultaneous of determination Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$

3.Investigation of complex formation between Fe (III) and thiocyanate.

References:

1.A. Finlay and J.A. Kitchener, Practical Physical Chemistry, Longman.

2.F. Daniels and J.H. Mathews, Experimental Physical Chemistry, Longman.

3.A.H. James, Practical Physical Chemistry, J.A. Churchil Ltd., 1961.

4.H.H. Willard, L.L. Merit and J.A. Dean, Instrumental Methods of Analysis, 4th Education, Affiliated East-West Press Pvt. Ltd., 1965.

5.D.P. Shoemaker and C.W. Garland, Experimental Physical Chemistry, McGrawHill.

6.J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publications, 1989

SECTION B

Use of Computational Chemistry softwares like pc GAMESS (firefly), Gaussian etc., to calculate molecular parameters.

Unit 7: Computational Chemistry Calculations

1.Single point energy calculations of simple molecules like H2O and NH3 at the HF/3-21G level of theory.

2.The effect of basis set on the single point energy of H2O and NH3 using the Hartree-Fock method (3-21G, 6-31G, 6-31+G, 6-31+G* basis sets can be used).

3.Geometry optimization of molecules like H2O, NH3, HCHO & C2H4 at the HF/6-31G level of theory.

4.Computation of dipole and quadrupole moments of HCHO & C2H4 at the HF/6-31G level of theory.

5.Effect of basis set on the computation of H-O-H bond angle in H2O using the Hartree- Fock method (3-21G, 6-31G, 6-31+G, 6-31+G* basis sets can be used).

6.Computation of the energy of HOMO and LUMO of formaldehyde and ethylene at the HF/6-31G level of theory.

7.Effect of substituent (F & Cl) on the geometric parameters (like C-C bond length) of ethylene at the HF/6-31G level of theory.

8.Comparison of stability of cis-planar and trans-planar conformers of H2O2 at the HF/6-31G level of theory.

9.Comparison of stability of cis- and trans- isomers of difluoroethylene at the HF/6-31G* level of theory.

10.Computation of the frequencies of normal modes of vibration of molecules like H2O, NH3 and CO2 at the HF/6-31+G* level of theory.

11.Determination of hydrogen bond strength of H2O dimer and H2O trimer at the HF/6-31+G* level of theory.

12.Determination of hydrogen bond strength of HF dimer and HF trimer at the HF/6-31+G* level of theory.

Reference:

1.J. Foresman &Aelieen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.

2.David Young, Computational Chemistry- A Practical Guide for Applying Techniques to Real- World Problems", Wiley -Interscience, 2001.

3.http://classic.chem.msu.su/gran/gamess/index.html

QP Code Reg. No.....

M.Sc Degree (C.S.S) Examination First Semester

Time: Three hours Max. Weightage: 30

Section- A

(Answer any eight questions. Each question carries 1 weightage)

1.What is synergism?

2. Define the term "isolobal".

3. Give an example for a β-elimination reaction.

4. What are Ziegler- Natta catalysts?

5. What is Bohr Effect?

6. What is cis-platin? What are its important applications?

7. What is radiation polymerisation?

8. How is nuclear reaction cross section related to reaction rate?

9. List the important functions of biological membranes.

10. Give an example for the use of palladium catalysts in the formation of C-N bond.

11. What is metathesis reaction?

12. Define hapticity with an example.

(8 x 1 = 8)

Section B

(Answer any four questions. Each question carries 3 weightage)

13. Discuss the bonding in ferrocene.

14. What are oxidative addition reactions? Discuss the important mechanisms involved in oxidative additions.

15. What is Wilkinson's catalyst? What are its uses? Describe alkene hydrogenation using Wilkinson's catalyst with the help of Tolman catalytic loops.

16. Explain the structure and functions of carbonic anhydrase, carboxypeptidase A and superoxide dismutase.

17. Write a note on the synthesis of transuranic elements.

18. Outline the role of chlorophyll in photosynthesis.

19.What are insertion reactions? Discuss insertion of alkenes and alkynes in the Ar-H bond.

(4 x 3 = 12)

Section C

(Answer any two questions. Each question carries 5 weightage)

20.What are π-bonding ligands? Explain the preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes.

21.a) Write a note on carbonylation reactions.

b) Write a note on asymmetric catalysis. Discuss asymmetric hydrogenation, isomerisation and epoxidation.

22.Discuss oxygen transport mechanism. What are the functions of haemoglobin and myoglobin in oxygen transport?

23.a) Discuss important analytical applications of radioisotopes.

b) Outline fluxional isomerism of allyl, cyclopentadienyl and allene systems.

(2 x 5 = 10)