M.E.S MAMPAD COLLEGE
Autonomous

M.Sc. DEGREE PROGRAMME
IN
CHEMISTRY

UNDER CREDIT AND SEMESTER SYSTEM

SCHEME AND SYLLABI

2021 ADMISSION ONWARDS

MES COLLEGE MAMPAD

M.Sc. CHEMISTRY (CSS PATTERN)

Regulations and Syllabus with effect from 2019 admission

The Board of Studies in Chemistry (PG) at its meeting held on 11-06-2019 considered the revision of M.Sc. Chemistry syllabus under Credit Semester System (CSS) and resolved to implement the revised syllabus from 2019 admission onwards. The revised programme pattern; syllabus, distribution of credits and scheme of evaluation, etc. approved by the Board of studies in Chemistry (PG) at its meeting held on 11-06-2019 are given below:

Pattern of the Programme

a) The name of the programme shall be M.Sc. Chemistry under CSS pattern.

b) The programme shall be offered in four semesters within a period of two academic years.

c) Eligibility for admission will be as per the rules laid down by the University from time to time.

d) Details of the programme offered for the programme are given in Table 1. The programme shall be conducted in accordance with the programme pattern, scheme of examination and syllabus prescribed. Of the 25 hours per week, 13 hours shall be allotted for theory and 12 hours for practical. 1 theory hour per week during even semesters shall be allotted for seminar.

Theory Courses

In the first three semesters there will be four theory courses and in the fourth semester three theory courses. All the theory courses in the first and second semesters are core courses. In the third semester there will be three core theory courses and one elective theory course. Colleges can choose any one of the elective courses given in table 1. In the fourth semester there will be one core theory course and two elective theory courses. Colleges can select any two of the elective courses from those given in table 1. However, a student may be permitted to choose any other elective course of his choice in the third and fourth semesters, without having any lecture classes. Of all the elective courses, one elective course in the third semester and two elective courses for the fourth semester chosen by the college only will be considered for calculating the workload of teachers. All the theory courses in the first, third and fourth semesters (both core and elective) are of 4 credits while the theory courses (both core and elective) in the third semester are of 3credits.

Practical Courses

In each semester, there will be three core practical courses. However the practical examinations will be conducted only at the end of second and fourth semesters. At the end of second semester, three practical examinations with the codes CHE1L01 & CHE2L04, CHE1L02 & CHE2L05 and CHE1L03 & CHE2L06 will be conducted. Practical examinations for the codes CHE3L07 & CHE4L10, CHE3L08 & CHE4L11 and CHE3L09 & CHE4L12 will be conducted at the end of fourth semester. Each practical examination will be of six hour duration and 3 credits. Three hours per week in the fourth semester are allotted for conducting individual project work by the students under the guidance of a faculty and it can be treated as practical hours while calculating the workload of teachers.

Project and Viva Voce

Each student has to perform an independent research project work during the programme under the guidance of a faculty member of the college/ scientists or faculties of recognised research institutions. Projects done in the quality control or quality analysis division of the industries will not be considered. At the same time, projects done in the R & D division of reputed industry can be considered. Each student has to submit three copies of the project dissertation for valuation at the end of fourth semester. After the valuation one copy may be returned to the student, one may be given to the project supervisor and the third one should be kept in the department/college library. Evaluation of the project work (4 credits) will be done on a separate day at the end of fourth semester, after the theory examinations. Viva voce on the project will also be done on the same day.

A comprehensive viva voce examination (2credits), based on all the theory and practical courses, will be conducted at the end of the fourth semester, on a separate day.

Grading and Evaluation

(1) Accumulated minimum credit required for the successful completion of the programme shall be 80.

(2) A project work of 4 credits is compulsory and it should be done during the programme. 3 hours per week are allotted in the IV semester, for carrying out the project work. Project evaluation should be conducted by three external examiners, one each from inorganic chemistry, organic chemistry and physical chemistry area, at the end of the fourth semester,

on a separate day. Also a comprehensive Viva Voce Examination (carrying 2 credits) may be conducted by three external examiners, one each from inorganic chemistry, organic chemistry and physical chemistry area, at the end of the fourth semester on a separate day.

(3) Evaluation and Grading should be done by direct grading system. All grading during the evaluation of courses and the semester is done on 6 point scale (A+, A, B, C, D, E). Grading in 6 point scale is as given below.

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

The calculation of GPA, SGPA & CGPA Shall be based on the direct grading system using 10 point scale as detailed below.

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

Pass in a course: P grade and above (GPA 2.00 and above). Pass in all courses in a semester is compulsory to calculate the SGPA.

GPA, SGPA and CGPA – between 0 to 5 and in two decimal points. An overall letter grade (Cumulative Grade) for the whole programme shall be awarded to the student based on the value of CGPA using a 10-point scale given below.

CGPA	Overall Letter Grade
4.25 – 5.00	O
3.75 – 4.24	A+
3.25 – 3.74	A
2.75 – 3.24	B+
2.50 – 2.74	B
2.25 – 2.49	C
2.00 -2.24	P
< 2.00	F
0	I
0	Ab

(4) Weightage of Internal and External valuation:

The evaluation scheme for each course shall contain two parts (a)) internal evaluation (b) external evaluation. Its weightages are as follows:

Evaluation	*Weightage*
Internal	1 (or20%)
External	4 (or80%)

Both internal and external evaluation will be carried out using Direct Grading System, in 6 points scale

(5) Internal evaluation (must be transparent and fair):

Theory: 5 weightage

a) Internal Examinations- weightage = 2 (1 internal exam)

b) Assignments and Exercises- weightage=1

c) Seminars/Viva Voce- weightage=1
d) Attendance - weightage=1

Practical: 10 weightage

a) Attendance - weightage=2
b) Lab. skill/quality of their results- weightage=2
c) Model practical test-weightage= 2 (Best one, out of two model exams is considered)
d) Record – weightage =2
e) Viva Voce- weightage=2

Project: 10 weightage

a) Literature survey and data collection-weightage=2
b) Interpretation of data & Preparation of Project report - weightage=2
c) Research attitude - weightage =2
d) Viva Voce- weightage=4

Project internal evaluation of each student should be done by the supervising faculty assigned by the department.

Viva Voce: No internal evaluation for viva voce examinations (at the end of 4th semester).

Attendance: Above 90%: A+, 85 – 89.99% : A, 80 – 84.99%: B, 75 -79.99%: C
70 – 74.99%: D, < 70%: E

(6) External evaluation:

a) **Theory**: In all semesters the theory courses have 30 weightage each.

Pattern of question Papers for theory courses is as follows

Division	*Type*	*No.of Questions*	*Weightage*	*Total Weightage*
Section A	Short Answer	8 out of 12	1	8
Section B	Short Essay	4 out of 7	3	12
Section C	Essay	2 out of 4	5	10
		Total weightage in a question paper		**30**

b) **Practicals**: At the end of II and IV semesters. There will be three practical examinations at the end of second semester as well as at the end of fourth semester.Each examination has 30 weightage and 3 credits

c) **Comprehensive Viva Voce**: At the end of IV semester on a separate day (2credits). Vivavoce will be based on both the theory and practical courses during the programme.

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**

c) **Project Evaluation**: End of IV semester on a separate day. Evaluation is based on:

a) Sigificance and relevance of the project-weightage=5
b) Project report - weightage=8
c) Presentation- weightage =5
c) Viva Voce- weightage =12

Total weightage 30 and credit for project is 4.

(7) Directions for question paper setters:

Section A: Set each questions to be answered in 5 minutes duration.

Section B: 20 minutes answerable questions each. May be asked as a single question or parts.

Section C: 30 minutes answerable questions each. May be asked as a single question or parts.

While setting the question paper, all units in each theory courses must be given due consideration and should give equal distribution as possible.

(Furthur details regarding the grading and evaluation are as per the University PG regulations 2019)

Jamsheer AM
HOD , Department of chemistry
Chairman, Board of Studies (ChemistryPG),
MES Mampad College

Audit courses:

Ability Enhancement Courses(AEC):

This course aims to have hands on experience for the students in their respective field of study, both in the core and elective subject area. Also it is a platform for the student community to have basic concepts of research and publication.

AEC is 4 credit course and should be conducted during the first semester of the programme. Credit of the AE course will not be considered while calculating the SGPA/CGPA. But the student has to obtain minimum pass requirements in this course, which is compulsory for overall pass in the programme

One particular AEC may be selected for all the students in a batch in the department or each student in a batch may choose one AEC, among the pool of courses suggested below. Either a single faculty from the department may be in charge of this course for a batch or each student may be assigned to a particular faculty in the department, in charge of this AEC, which will be decided by the department council/ HoD.

a) Industrial/Research institution visit/visits
b) Publication of a research article/articles in national/international journal
c) Presentation of research paper/papers in national level seminar/conference, which should be published in the seminar/conference proceedings
d) Review article/articles on research topics which is presented in a national level seminar/conference and published in the proceedings
e) Internships at any reputed research institutions/R&D centre/Industry

After conducting the AEC, the evaluation/examination should be done either common for all students in a batch or individually depending upon the AEC conducted. The evaluation/ examination must be conducted jointly by the teacher in charge of the AEC and the head of the department. The result of the AEC, duly signed and sealed by both teacher in charge and head of the department, should be uploaded to the University during the stipulated time period in the third semester of the programme. Evaluation/examination must be conducted by 30 weightage pattern, as in the theory courses and the GPA and overall grade of the AEC should be uploaded to the University. Evaluation/examination on AEC must contain the following components: MCQ type written examination, Report on AEC, Presentation of AEC, Viva voce on AEC. Distribution of 30 weightage may be done by the teacher in charge in concurrence with the Head of the department.

Professional Competency Course (PCC):

This course particularly aims to improve the skill level of students, especially for using specific as well as nonspecific software useful in their respective field of study, both related to the core and elective subject area. Also, it is a platform for the student community to undertake socially committed projects and thereby developing a method of leaning process by through the involvement with society. PCC is a 4-credit course and should be conducted during the second semester of the programme. The credit of the PC course will not be considered while calculating the SGPA/CGPA.

But the student has to obtain minimum pass requirements in this course, which is compulsory for an overall pass in the programme One particular PCC may be selected for all the students in a batch in the department or each student in a batch may choose one PCC, among the pool of courses suggested below. The exact title of the course may be decided by the department, but the area of study should be from the pool of courses suggested below. Either a single faculty from the department may be in charge of this course for a batch or each student may be assigned to a particular faculty in the department, in charge of this PCC, which will be decided by the department council/ HoD.

a) Development of skills on using softwares like Gaussian, Gamessetc which is useful in molecular modeling, drug designing, etc.

b) Development of skills on using softwares like Chemdraw, Chemwindow, ISIS draw, etc which is useful in drawing purposes, structural predictions, etc.

c) Training on computational chemistry

d) Case study and analysis on any relevant issues in the nearby society(for example water analysis, soil analysis, acid/alkali content analysis, sugar content analysis, etc)

e) Any community linking programme relevant to the area of study(For example Training for society on soap/perfume making, waste disposal, plastic recycling, etc)

After conducting the PCC, the evaluation/examination should be done either common for all students in a batch or individually depending upon the PCC conducted. The evaluation/ examination must be conducted jointly by the teacher in charge of the PCC and the head of the department. The result of the PCC, duly signed and sealed by both teacher in charge and head of the department, should be uploaded to the University during the stipulated time period in the third semester of the programme. Evaluation/examination must be conducted by 30 weightage pattern, as in the theory courses and the GPA and overall grade of the PCC should be uploaded to the University. Evaluation/examination on PCC must contain the following components: MCQ type written examination, Report on PCC, Presentation on PCC, Viva voce on PCC. Distribution of 30 weightage may be done by the teacher in charge in concurrence with the Head of the department

TABLE 1
Courses offered for M.Sc. Chemistry Programme under CSS Patten in Affiliated Colleges (2019 onwards)

Semester	Course Code	Course Title	Instruction/ Week	Credits
I	CHE1C01	Quantum Mechanics and Computational Chemistry	4	4
	CHE1C02	Elementary inorganic chemistry	3	4
	CHE1C03	Structure and reactivity of organic Compounds	3	4
	CHE1C04	Thermodynamics, kinetics and catalysis	3	4
	CHE1L01	Inorganic chemistry practical I	4	-
	CHE1L02	Organic chemistry Practical I	4	-
	CHE1L03	Physical chemistry practical I	4	-
		Total credits:	**Core**	**16**
II	CHE2C05	Group theory and Chemical Bonding	3	3
	CHE2C06	Coordination chemistry	3	3
	CHE2C07	Organic reaction mechanisms	3	3
	CHE2C08	Electrochemistry, solid state chemistry and Statistical Thermodynamics	3	3
	CHE2L04	Inorganic chemistry practical II	4	3
	CHE2L05	Organic chemistry practical II	4	3
	CHE2L06	Physical chemistry practical II	4	3
		Total credits:	**Core**	**21**
III	CHE3C09	Molecular spectroscopy	4	4
	CHE3C10	Organometallic &Bioinorganic chemistry	3	4
	CHE3C11	Reagents and Transformations in Organic Chemistry	3	4
	CHE3L07	Inorganic chemistry practical III	4	
	CHE3L08	Organic chemistry practical III	4	
	CHE3L09	Physical chemistry practical III	4	
	CHE3E01	Synthetic organic chemistry(Elective)	3	4
	CHE3E02	Computational chemistry(Elective)	3	4
	CHE3E03	Green and Nanochemistry(Elective)	3	4
		Total Credits:	**Core** **Elective**	**12** **4**

	CHE4C12	Instrumental Methods of Analysis	4	4
	CHE4L10	Inorganic Chemistry Practical IV	3	3
	CHE4L11	Organic Chemistry Practical IV	3	3
	CHE4L12	Physical Chemistry Practical IV	3	3
	CHE4E04	Petrochemicals and Cosmetics(Elective)	4	4
	CHE4E05	Industrial Catalysis(Elective)	4	4
	CHE4E06	Natural Products & Polymers(Elective)	4	4
	CHE4E07	Material Science(Elective)	4	4
	CHE4E08	Organometallic Chemistry	4	4
	CHE4P01	Research Project	3	4
	CHE4V01	Viva Voce		2
		Total Credits: **Core** **Elective** **Project** **Viva**		 **13** **8** **4** **2**
TOTAL CREDITS OF THE PROGRAMME		**CORE** **ELECTIVE** **PROJECT** **VIVAVOCE** ***TOTALCREDITS***		**62** **12** **4** **2** **80**

Syllabus Year	2021-2022
Department	Chemistry
Programme	MSc chemistry

Programme outcome.

Sl.No	Programme Outcome
PO1	Gains complete knowledge about all fundamental aspects of chemistry covering all process and prospectives
P02	Familiarize with all branches and the emerging areas of chemistry and their applications in various spheres of sciences expose the diversified aspects of chemistry where the students experience a broader outlook of the subject.
PO3	Student will be able to handle standard and modern scientific instruments and acquire analytical skills to synthesize the chemical compounds by maneuvering the addition of reagents under optimum reaction conditions
PO4	Able to solve complex chemical problem such as analysis of data, synthetic logic, spectroscopy, structure and modeling, which are essential skills to succeed in field of research or in industry.

Programme specific out come

Sl.No	Programme Specific Outcome.
1	Understand the theoretical and physical aspects of atomic structure, chemical bonding, reaction pathways and dynamics, various energy transformations, molecular assembly in nano level, significance of electrochemistry, molecular segregation using their symmetry
2	Familiarize various reagents for organic synthesis, organic reaction mechanisms, separation techniques, stereochemistry etc
3	Identify the principles, structure and reactivity of organic and inorganic compounds (complexes) and able to characterize materials and interpret their spectra
4	Obtain knowledge in qualitative and quantitative techniques and contribute new scientific insights or innovative applications of chemical research to the next generation
5	Understand and apply the tools and concepts of computational quantum chemistry methods to the problems of chemistry and other branch of science

Course Outcome

Semester	Course Code	Course Name	Course out come
I	**CHE1C01**	**QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY**	The students are expected to
			1. Understand the historical background, evolution, importance and impact of quantum mechanics in science

			2. Understand the basic concepts and postulates of quantum mechanics
			3. Apply concept of quantum mechanics to exact solvable systems of translational, rotational and vibrational motions
			4. Apply concept of quantum mechanics to atomic structure and chemical bonding and realize that the wave functions of hydrogen atom are nothing but atomic orbitals and understand that chemical bonding is the mixing of wave functions of the two combining atoms.
			5. Familiarize approximation methods of quantum mechanics and apply those methods to many electron atoms
			6. Understand and apply the tools and concepts of computational quantum chemistry methods to the problems of chemistry
			7. Inculcate an atomic/molecular level philosophy in the mind.
	CHE1C02	Elementary inorganic chemistry	The students will be able to
			1. Understand the basic principles of acid – base chemistry and non – aqueous solvents
			2. Understand the chemistry of the main group, transition and inner transition elements.
			3. Understand nuclear fission, fusion and radiation chemistry .
			4. Know the significance of nanoscale & its dimensions
			5. Acquire knowledge of various characterization techniques and the short term and longer term applications of nanomaterials.
	CHE1C03	Structure and reactivity of organic Compounds	1.Able to identify aromaticity,non aromaticity and anti aromaticity of compounds and to predict their stability.
			2.To propose reaction mechanisms and determine

			neighbouring group participation effects on rates of reactions
			3.Students will be able to evaluate the stability of various conformations of cyclic and acyclic systems using steric,electronic and stereo electronic effects and correlate them to reactivity
			4.Acquire knowledge about the importance of asymmetric synthesis and will be able to propose synthesis of molecules of reasonable complexity with the control of
			stereo chemistry
	CHE1C04	Thermodynamics, kinetics, and catalysis	1 • Understand the terminologies associated with thermodynamics and fundamental relations in irreversible thermodynamics
			2.Understand the theories and methods of determination of the kinetics of the fast reaction.
			3 .Knowledge of molecular reaction dynamics.
			4.Knowledge of homogeneous and heterogeneous catalysis and the related mechanisms.
II	CHE2C05	Group theory and Chemical Bonding	The students are expected to
			1. Understand the basic concepts of group theory and apply group theory concepts and character table to various chemical applications
			2. Analyze various symmetry operations of molecule and predict the symmetry and point group of molecules.
			3. Familiarize character table and apply character table as a tool for the prediction of IR and Raman active vibrational modes and prediction of electronic spectra
			4. Apply character table for the finding orbitals for hybridization and generation of SALCS
			5. Understand quantum

			mechanical concepts of hybridization and bonding of polyatomic molecules.
	CHE2C06	Coordination chemistry	1.Enable student to understand the stability of coordination compounds and their bonding characters
			2.Understand the spectral properties of coordination compounds
			3.Understand the reactions and their mechanism in coordination compounds
			4.Enable student to understand the redox and photochemical reactions in coordination compounds.
	CHE2C07	Organic reaction mechanisms	1.Understand the mechanism of different organic reactions.
			2.Students will be able to predict the product and mechanism of different reactions.
			3.The intermediates formed during various organic reactions can be identified.
			4.The students will be able to explain different name reactions of carbonyl compounds.
			5. Will enable the students to predict the out put of click chemistry.
			6.The students will acquire proper knowledge about photochemical reactions with mechanism
			7.The students will understand the chemistry of natural products including biosynthesis
	CHE2C08	Electrochemistry, solid state chemistry and Statistical Thermodynamics	Students will be able to
			1.Understand the chemistry of electrochemical cells, fuel cells and dynamic electrochemistry.
			2. Understand symmetry elements, symmetry operations and crystal systems.
			3. know the stoichiometric and non stoichiometric defects in crystals.
			4. Understand Maxwell Boltzman, Bose-Einstein and Fermi-Dirac statistics and their

			applications.
			5. Know the classical and quantum theories of heat capacities of solids
II (Practical)	CHE1L01&CHE2L04	Inorganic chemistry practical I & Inorganic chemistry practical II*	1.To enable the students to develop skill in the qualitative determination of common and less common cations from their mixture
			2.To understand the theory of colorimetry and the way of determining the quantity of metal ions through this technique.
			3. To enable the students to develop skill in the cerimetric determination of metal ions
			4.To apply proper techniques for volumetric estimation of metal ions
	CHE1L02&CHE2L05	Organic chemistry Practical I & Organic chemistry Practical II*	1.Able to identify the functional groups present in the given organic compound
			2.To learn the pilot separation of bi mixtures
			3.To understand the techniques involving drying and recrystallisation of synthesised organic compounds by various methods and to determine their b.p&m.p
			4.Able to synthesise solid derivatives of all organic compounds with different functional groups
	CHE1L03&CHE2L06	Physical chemistry practical I & Physical chemistry practical II*	The students are expected to
			1.Acquire analytical skills for measuring physical parameters
			2.Understand the basic principle and applications of conductometric ,potentiometric,refractometric and viscosity measurements
			3.Acquire skills for handling instruments like conductivity meter ,potentiometer,refractometer etc
			4. Construct phase diagram for two component systems
			5.Calculate thermodynamic parameters from thermochemistry experimental data
III			The students are expected to

	CHE3C09	Molecular spectroscopy	1. Understand the theoretical background of various spectroscopic techniques.
			2. Understand the fundamentals of UV, IR, NMR and mass spectroscopy for the characterization of organic molecules.
			3. Use combined spectral data of various techniques for the structural elucidation of organic compounds
			4. Apply spectroscopic methods as analatytical tool for characterization of materials in chemistry, biology, and medicine and material science
	CHE3C10	Organometallic And Bioinorganic chemistry	1.Acquire knowledge about the nature of ligands, its electron donating ability and bonding modes of ligands with metal ions.
			2.Able to understand the stability and structural patterns of metal clusters,carbonyls and nitrosyls.
			3.Able to identify the role of metal ions in the biological and physiological systems and applications.
			4.Get knowledge about the homogeneous and heterogeneous organometallic catalysts in various industrial processes.
	CHE3C11	Reagents and Transformations in Organic Chemistry	1.students are expected to understand the reagents used for oxidation and reductions
			2.Students will be able to design the mechanisms of organic reactions.
			3.students will acquire knowledge of supramolecular chemistry and type of interactions between molecules.
			4.students will be able to identify selective reagents used for oxidation reactions
	CHE3E01	Synthetic organic chemistry (Elective)	1.Students acquire proper knowledge on various reagents used for organic synthesis.
			2.Students can predict the

			products formed when different reagents are used in a reaction.
			3.Students can evaluate the use of different reagents for various reactions.
			4.Students acquire proper knowledge on carbonyl compounds.
			5.Students understand the use and applications of different coupling reactions.
			6/Students will be able to plan, design and expain the mechanism of synthesis of different organic compounds.
			7.Students will be able to identify the synthons, synthetic equivalents, synthetic reagents and substrates required for a reaction leading to a particular product.
			8.Students will acquire knowledge on synthesis, reactions and applications of heterocyclic compounds
IV	CHE4C12	Instrumental Methods of Analysis	Students will be able to;
			1.understand the principles of conventional procedures
			2.Evaluate errors in measurements and to minimise errors while conduction of measurements.
			3.Identify compounds from a mixture using chromatographic techniques.
			4. Understand principle and procedures of optical amd electroanalytical methods
	CHE4E06	Natural Products & Polymers(Elective)	1.Acquire knowledge of the classification of the natural products by their molecular structures and biosynthesis.
			2.Aqcuire knowledge of the functions of important natural products and the methodology used in natural product chemistry
			4.Get a comprehensive knowledge about different

			polymerization techniques and characterizations.
			5.Can interpret the stereochemistry of polymers and the knowledge of optoelectronic properties of polymers and their application in to electronic research
	CHE4E08	Organometallic Chemistry (Elective)	1.Able to identify the structure and bonding aspects of simple organometallic compounds.
			2.Apply different electron counting rules to predict the shape/geometry of low and high nuclearity metal carbonyl clusters
			3. Identify the different types of organometallic reactions and apply the above concepts to explain different catalytic reactions
			4.Able to understand fundamental reaction types and mechanisms and how to combine these to understand efficient catalytic processes in small scale and large scale by homogeneously/heterogeneously
IV (practical)	CHE3L07& CHE4L10	Inorganic chemistry practical III & Inorganic chemistry practical	The students will be able to
			1. Quantitatively separate and estimate ions in a binary mixture using volumetric,gravimetric and colorimetric techniques.
			2.Understand solvent extraction technique.
			3.Expertise in Ion- exchange separation and estimation of binary mixtures
			4.Prepare inorganic complexes.
	CHE3L08& CHE4L11	Organic chemistry Practical III & Organic chemistry Practical IV	1.Students develop skill in the estimation of reducing sugar, amino group, phenolic group and esters volumetrically.
			2.Students develop skill in the estimation of vitamin C, drugs and anti-biotics colorimetrically.
			3.Students develop skill in the estimation the extraction of natural products and purification by column chromatography and TLC

			4.Students develop skill in the prepartion of chromatographic plate and chromatographic paper for the separation and identification of various organic compounds.
			5. Students develop skill in theTLC plate activation and identification of compoundsdyes, food additives, food colours, amino acids, sugars, pesticides and herbicides
	CHE3L09& CHE4L12	Physical chemistry practical III & Physical chemistry practical IV	The students are expected to
			1.Verify experimentally the fundamental concepts related to kinetics
			2.Understand ,apply and verify various adsorption isotherms related to adsorption from solution
			3. Construct phase diagram for three components systems
			4. familaralize computational chemistry programme firefly and apply the programmes for the calculation of energy ,prediction of geometry,frequency etc

M E S COLLEGE MAMPAD - AUTONOMOUS
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I
CHE1C01-QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY
(4Credits, 72 hours)

		L	C
CHE1C01	Quantum Mechanics and Computational Chemistry	4	4
Objectives	1.Introduce basic and advanced concepts and postulates of quantum mechanics 2. Enable the students to solve Schrodinger equation for translational ,vibrational ,rotational motions and hydrogen like atoms. 3.Give a glimpse of various approximation methods and computational quantum chemistry methods and familiarize the students different computational methods and programmes		
Course outcomes	The students are expected to 1. Understand the historical background, evolution, importance and impact of quantum mechanics in science 2. Understand the basic concepts and postulates of quantum mechanics 3. Apply concept of quantum mechanics to exact solvable systems of translational, rotational and vibrational motions 4. Apply concept of quantum mechanics to atomic structure and chemical bonding and realize that the wave functions of hydrogen atom are nothing but atomic orbitals and understand that chemical bonding is the mixing of wave functions of the two combining atoms. 5. Familiarize approximation methods of quantum mechanics and apply those methods to many electron atoms 5. Understand and apply the tools and concepts of computational quantum chemistry methods to the problems of chemistry 6. Inculcate an atomic/molecular level philosophy in the mind.		

Unit 1: Introduction to Quantum Mechanics (9hrs)

Failures of classical mechanics and historical background of quantum mechanics - Black body radiation and Planck's quantum postulate. Photoelectric effect, atomic spectra, Compton effect .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 (9hrs)

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 (9hrs)

Co-ordinate systems: - Cartesian, and spherical polar coordinates and their relationships. Planar rigid rotor (or particle on a ring), the Phi-equation, solution ofthe 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.

Operators corresponding to angular momenta ((Lx, Ly, Lz), commutation relations between these operators, Angular momentum in spherical polar co-ordinate, space quantization. Spherical harmonics as Eigen functions of angular momentum operators Lz and L^2. Ladder operators.

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

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.

Quantum numbers. The postulate of spin by Uhlenbeck and Goudsmith, Dirac's relativistic equation for hydrogen atom and discovery of spin (qualitative treatment), Stern – Gerlach, experiment spin orbitals, construction of spin orbitals from orbitals and spinfunctions.

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

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 of hydrogen atom using trial function e^{-ar}. 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 (9hrs)

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).Vector model atom. Atomic term symbols

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

Electronic structure of molecules – Basics of HF-SCF method of molecules(derivation not required) Hartree-Fock limit. Post Hartree-Fock methods - introduction to Møller Plesset perturbation theory, configuration interaction, coupled cluster and semi empirical methods

Classification of Computational Chemistry methods – Molecular mechanics methods (concept of force field) and Electronic structure methods, ab initio and semi-empirical methods (Basic idea only), Density Functional Theory Hohenberg-Kohntheorems,Kohn-Sham orbitals,

Comparison of ab initio, semi empirical and DFT methods.

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

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 key words, Specification of molecular geometry using a) Cartisian coordinates and b) Internal coordinates. The Z-matrix - Z- matrices of some simple molecules like H_2,H_2O, formaldehyde, ammonia ,methanol, formaldehyde , Ethane – eclipsed & staggered conformations.

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1. F.L. Pilar, *Elementary Quantum Chemistry* , McGraw-Hill,1968.
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Reference (for units 7 & 8)

1. C. J. Cramer, *Essentials of computational Chemistry: Theories and models*, John Wiley & Sons 2002.
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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.
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M E S COLLEGE MAMPAD - AUTONOMOUS

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I CHE1C02 - - ELEMENTARY INORGANIC CHEMISTRY (4 Credits, 54hrs)

CHE1C02	Elementary inorganic chemistry	L	C
		3	4
Objectives	To make the students conversant with the basic concept of acids and bases, chemistry of the main group, transition and inner transition elements, nuclear and radiation chemistry, definition and significance of nanoscale materials, different methods of preparation of nanomaterials, various tools for characterizing nanomaterials.		
Course outcomes	The students will be able to 1. Understand the basic principles of acid – base chemistry and non – aqueous solvents 2. Understand the chemistry of the main group, transition and inner transition elements. 3. Understand nuclear fission, fusion and radiation chemistry . 4. Know the significance of nanoscale & its dimensions 5. Acquire knowledge of various characterization techniques and the short term and longer term applications of nanomaterials.		

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

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.-theoretical basis of hardness and softness. The Drago-Wayland equation, E and C parameters-Symbiosis. Applications of HSABconcept.

Chemistry of nonaqueous solvents- NH_3, SO_2, H_2SO_4, BrF_3, HF, N_2O_4 and HSO_3 F. Nonaqueous solvents and acid-base strength. Super acids –surface acidity. Application of super acids.

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

Chemical periodicity-First and Second raw anomalies-The diagonal relationship- Periodic anomalies of the nonmetals and post-transitionmetals.

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 and hypo 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(9hrs)

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 (9hrs)

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 (of lanthanides and actinides). Uranyl compounds. Trans-actinide elements. Super heavy elements – production and chemistry.

Unit 5: Nuclear and Radiation Chemistry (9hrs)

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-radiationdosimetry.

Unit 6: Chemistry of Nanomaterials (9hrs)

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. Scaning prob microscopies-STM, AFM. X-ray photoelectron spectroscopy(XPS), Dynamic light scattering(DLS), X-ray diffraction(XRD).

Applications: Nanoelectronics, nanosensors, nanocatalysts, nanofilteration, diagnostic and therapeutic applications and targeted drug delivery.

Introduction to graphenes and fullerenes.

Reference (for units 1 to 5)

1. N.N. Greenwood and A.Earnshaw, *Chemistry of Elements*, *2/e*, *Elsevier* Butterworth- Heinemann,2005.
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Reference (for unit 6):

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M E S COLLEGE MAMPAD - AUTONOMOUS

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

CHE1C03 - STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS

(4 Credits, 54hrs)

CHE1C03	Structure and reactivity of organic Compounds	L 3	C 4
Objectives	1.To introduce the concept of aromaticity and effect of structure on reactivity of organic compounds 2. To understand different conformations,their stabilities and reactions of cyclic and acyclic compounds 3.To learn the prochirality and chirality at centers,planes and helices and determine the absolute configuration 4.To impart the various aspects of asymmetric synthesis such as basic principles of enantio selective reactions,dynamic and kinetic transformations		
Course outcomes	1.Able to identify aromaticity,non aromaticity and anti aromaticity of compounds and to predict their stability. 2.To propose reaction mechanisms and determine neighbouring group participation effects on rates of reactions 3.Students will be able to evaluate the stability of various conformations of cyclic and acyclic systems using steric,electronic and stereo electronic effects and correlate them to reactivity 4.Acquire knowledge about the importance of asymmetric synthesis and will be able to propose synthesis of molecules of reasonable complexity with the control of stereo chemistry		

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

Nature of Bonding in Organic Molecules: Localized and delocalized chemical bonding, bonding weaker than 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 heteroannulenes, fused ring systems, fulvenes, fulvalenes, azulenes, pentalenes and heptalenes. Preparation of aromatic and antiaromatic compounds by different methods, stability of benzylic cations and radicals. Effect of delocalized electrons on pKa.

Unit 2: Structure and Reactivity (9hrs)

Transition state theory, Potential energy vs reaction co-ordinate curve, substituent effects (inductive, mesomeric, inductomeric, electomeric and field effects) on reactivity. Qualitative study of substitution effects in S_N1-S_N2 reactions. Neighbouring group participation, 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 (9hrs)

Factors affecting the conformational stability of molecules – dipole interaction, bond opposition strain, bond angle strain. Conformation of acyclic compounds – Ethane, n- butane, alkene dihalides, glycols, chlorohydrines, 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. Conformation of substituted cyclohexanone, 2-bromocyclohexanone, dibromocyclo hexanone, (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 substituent is 1-butyl and their importance in assessing the reactivity of an axial or equatorial substituent.

Unit 4: Conformational Analysis – II (9 hrs)

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-amino ethanol. (c) dehydro halogination of stilbene dihalide (dl and meso) and erythreo threo- bromo-1,2-diphenyl propane.

Effect of conformation on the course andrate of reactions in cyclohexane systems illustrated by: (a) S_N2 and S_N1 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 asequatorial carboxyl groups and hydrolysis of their esters. (g) Hydrolysis of axial and equatorialtosylates. (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 (9hrs)

Unit 5: Stereochemistry (9hrs)

Optical isomerism of compounds containing one or more asymmetric carbon atoms Pro chirality/Pro stereoisomerism, Prochiral centre, Prochiral molecules, Homo topic and heterotopic ligands and faces, substitution – addition criterion and symmetry criterion enantiotopic, diastereotopic and homotopic hydrogen atom, Pro-R, Pro-S, Re and Si nomenclature.

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 folding of helical structures

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, inter conversion of geometrical isomers. Methods of determination of the configuration of geometrical isomers in acyclic acid cyclic systems, stereochemistry of aldoximes and ketoximes

Unit 6: Asymmetric Synthesis (9 hrs)

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-Anhmodel.

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 IPC_2BH and $IPCBH_2$. Reduction with CBH reagent. Stereochemistry of Sharpless asymmetric epoxidation and dihydroxylation

4. Asymmetric aldol reaction: Diastereoselective aldol reaction and its explanation by Zimmermann-*Traxler* model. Auxillary controlled aldol reaction. Double diastereoselection-matched and mismatched aldol reactions

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M E S COLLEGE MAMPAD - AUTONOMOUS

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

CHE1C04 – THERMODYNAMICS, KINETICS AND CATALYSIS

(4 Credits, 54hrs)

CHE1C04	Thermodynamics, kinetics, and catalysis	L	C
		3	4
Objectives	To introduce the principles of chemical thermodynamics, kinetics, and catalysis and also to emphasize the advanced theories related to them		
Course outcomes	1 • Understand the terminologies associated with thermodynamics and fundamental relations in irreversible thermodynamics 2Understand the theories and methods of determination of the kinetics of the fast reaction. 3 Knowledge of molecular reaction dynamics. 4.Knowledge of homogeneous and heterogeneous catalysis and the related mechanisms.		

Unit 1: Thermodynamics (9hrs)

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 hrs).

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 hrs)

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 hrs)

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, Stripping and rebound mechanism 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 hrs)

Structure and chemical nature of surfaces, Adsorptionat 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 (9hrs)

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-precipitaion 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.

Reference:

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2 Keith J. Laidler, *Chemical Kinetics 3rd edn*., Pearson Education, 1987(Indian reprint 2008).

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15. Jens Hajen, *Industrial Catalysis: A Practical Approach.* 2nd Edn., Wiley VCH,2006.

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17. C.H. Bartholomew and R.J. Farrauto, *Fundamentals of Industrial Catalysis Process,* 2nd Edn. Wiley & Sons Inc.2006.

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M E S COLLEGE MAMPAD - AUTONOMOUS

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

CHE2C05 - GROUP THEORY and CHEMICAL BONDING (3 Credits, 54hrs)

		L	C
CHE2C05	Group theory and Chemical Bonding	3	3
Objectives	Introduce basic concepts of symmetry and group theory. Familiarize the students with different areas of character table and applications of group theory for bonding and spectroscopy. Introduce quantum mechanical treatment of hybridization and bonding in polyatomic molecules		
Course out comes	The students are expected to 1. Understand the basic concepts of group theory and apply group theory concepts and character table to various chemical applications 2. Analyse various symmetry operations of molecule and predict the symmetry and point group of molecules. 3. Familiarize character table and apply character table as a tool for the prediction of IR and Raman active vibrational modes and prediction of electronic spectra 4. Apply character table for the finding orbitals for hybridization and generation of SALCS 5. Understand quantum mechanical concepts of hybridization and bonding of polyatomic molecules.		

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

Basic principles of group theory - the defining properties of mathematical groups, finite and infinite groups, Abelian Isomorphic 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, Determination of point groups of molecules and ions (organic / inorganic / complex) belonging to Cn, Cs, Ci, Cnv, Cnh, C∞v, Dnh, D∞h, Dnd, Td and Oh point groups.

GMTof pointgroups for C2V , C3V and C2h

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

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., $\square_{cart}$) 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 (9hrs)

Molecular vibrations - symmetry species of normal modes of vibration, construction of □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. group theoretical explanation, relaxation in selection rules and distortion .

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

Hybridisation - 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 proj ection operator, use of projection operator in constructing SALCs for the MOs in cyclopropenyl ($C_3H_3^+$)cation. construction of symmetry adapted linear combination of atomic orbitals (SALCs) of C2v, C3v, D3h and C2h molecules.

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

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 hetero nuclear 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 (9hrs)

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 distributions 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)

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9. K.Veera Reddy, *Symmetry & Spectroscopy of Molecules 2nd Edn.*, New Age International 2009.

10.A.W. Joshi, *Elements of Group Theory for Physicists*, New Age International Publishers, 1997.

Reference(for units 5 &6)

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3. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics*, 4th Edition, Oxford University Press,2005.
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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.
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M E S COLLEGE MAMPAD - AUTONOMOUS

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

CHE2C06 - CO-ORDINATION CHEMISTRY (3Credits, 54hrs)

CHE2C06	Coordination chemistry	L	C
		3	3
Objectives	To introduce the bonding concepts in coordination chemistry and the study of properties and reactions of coordination compounds and their spectroscopic studies.		
Course out comes	1.Enable student to understand the stability of coordination compounds and their bonding characters 2.Understand the spectral properties of coordination cmpounds 3.Understand the reactions and their mechanism in coordination compounds 4.Enable student to understand the redox and photochemical reactions in coordination compounds.		

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

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 electrochemical method and spectrophotometry. Stabilisation 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 (9hrs)

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, tetragonal, linear and triagonal bipiramidal fields. Factors affecting crystal field splitting. Consquences of crystal eield 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 with and without π boning

Unit 3: Electronic Spectra and Magnetic Properties of Complexes (9hrs) Spectroscopic ground state. Terms of d^nconfigurations. Selection rules for d-d transitions, break down of selection rules. 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.The μ_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 Gouymethod.

Unit 4: Characterization of Coordination Complexes (9hrs)

Infrared spectra of metal complexes. Group frequency concept. Changes in ligand vibrations on coordination- metal ligand vibrations. Application in coordinationcomplexes. ESR spectra – application to copper complexes. NMR spectroscopy for structural studies of 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 (9hrs)

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 (9hrs)

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 redoxreactions.

Photochemical reactions of metal complexes- Prompt and delayed reactions. Exited 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 isomerisation and photo recimization. Illustration of reducing and oxidizing character of $[Ru(bipy)_3]^{2+}$ in the excited state. Metal complex sensitizers- water photolysis.

References:

1. N.N.Greenwood and A.Earnshaw, *Chemistry of Elements, 2/e,* Butterworth- Heinemann, 2005.

2 J.E.Huheey, E.A.Keiter, R.L.Keiter and 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.A.W.Adamson and P.D.Fleischauer, *Concepts of Inorganic Photochemistry,Wiley.*

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11.A.Earnshaw, *Introduction to Magnetochemistry, Academic Press,1968.*

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13.A.E. Martell, *Coordination Chemistry, Vol.I*

14.R.S. Drago, *Physical Methods in Inorganic Chemistry*, Affiliated East- West Press Pvt. Ltd.,1977

M E S COLLEGE MAMPAD - AUTONOMOUS

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

CHE2C07 - REACTION MECHANISM IN ORGANIC CHEMISTRY

(3 Credits, 54hrs)

CHE2C07	Organic reaction mechanisms	L 3	C 3
Objectives	1. To impart advanced knowledge of different organic reaction mechanisms, photochemistry, pericyclic reactions and reactive intermediates. 2. To introduce the different reactions of carbonyl compounds. 3. To develop knowledge on the chemistry of natural products		
Course out comes	1. Understand the mechanism of different organic reactions. 2. Students will be able to predict the product and mechanism of different reactions. 3. The intermediates formed during various organic reactions can be identified. 4. The students will be able to explain different name reactions of carbonyl compounds. 5. Will enable the students to predict the out put of click chemistry. 6. The students will acquire proper knowledge about photochemical reactions with mechanism 7. The students will understand the chemistry of natural products including biosynthesis.		

Unit 1: Aliphatic and Aromatic Substitutions (9 hrs)

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 bezylic substitutions. Ambident nucleophiles and substratesregioselectivity.

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 nucleophilicsubstitution.

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

(i) Addition and Elimination Reactions (6hrs)

Mechanistic and stereochemical aspects of addition toC=C involving electrophiles, nucleophiles and free radicals. Effect of substituents on 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 andCO_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 (9hrs)

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

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 Oppenaueroxidation.

Addition tocarbon-nitrogen multiple bond: Ritter reaction and Thorpe condensation. Hydrolysis, alcoholysis and reduction of nitriles.

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

Unit 4: Pericyclic Reactions (9 hrs)

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 hrs)

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, photodimerisation of α, β-unsaturated ketones,

Photo rearrangemets: Photo –Fries, di-π- methane, lumiketone, oxa di-π-methane rearrangements. Barton and Hoffmann-Loeffler-Freytag reactions. Photo isomerisation and dimerisation of alkenes, photo isomerisation 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.

2. F. A. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A & B*, 5/e, Springer,2007.

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7. S. Sankararaman, *Pericyclic Reactions-A Textbook: Reactions, Applications and Theory*, Wiley VCH,2005.

8. I. Fleming, *Molecular Orbitals and Organic Chemical Reactions*, Wiley,2009.

9. J. Sing and J. Sing, *Photochemistry and Pericyclic Reactions*, 3/e, New Age International,2012.

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11. M. B. Smith, *Organic Chemistry: An Acid Base Approach*, CRC Press,2010.

12. T. Okuyama and H. Maskill, *Organic Chemistry A Mechanistic Approach*, Oxford University Press,2014.

13. I. Fleming, *Selected Organic Synthesis*, John Wiley and Sons,1982.

14. T. Landbery, *Strategies and Tactics in Organic Synthesis*, AcademicPress, London,1989.

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 E S COLLEGE MAMPAD - AUTONOMOUS

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

CHE2C08 - ELECTROCHEMISTRY, SOLID STATE CHEMISTRY AND STATISTICAL THERMODYNAMICS (3 Credits, 54hrs)

CHE2C08	Electrochemistry, solid state chemistry and Statistical Thermodynamics	L 3	C 3
Objectives	To make the student familiar with the concepts of electrochemistry, solid state and statistical thermodynamics		
Course out comes	Students will be able to 1.Understand the chemistry of electrochemical cells, fuel cells and dynamic electrochemistry. 2. Understand symmetry elements, symmetry operations and crystal systems. 3. know the stoichiometric and non stoichiometric defects in crystals. 4. Understand Maxwell Boltzman, Bose-Einstein and Fermi-Dirac statistics and their applications. 5. Know the classical and quantum theories of heat capacities of solids		

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

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-Hückel equation,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 insolution

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 secondarycells.

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 (9hrs)

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 wavepotential.

Corrosion-Evans Diagram

UNIT 3: Solid State – I (9hrs)

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 glide planes, introduction to space groups.

Bragg's law and applications, lattice planes and miller indices, *d*-spacing formulae, crystal densities and unit cellcontents,

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

UNIT 4: Solid State – II (9hrs)

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 & specificheat

Unit 5: Statistical Thermodynamics- I (9hrs)

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, Maxwell- Boltzman 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 diatomicgases.

Unit 6: Statistical Thermodynamics- II (9hrs)

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-Boltzman, Bose-Einstein, and Fermi-Dirac statistics.

Reference:

For Units 1-4

1. D. R. Crow, *Principles and Applications of Electrochemistry*, Chapman and Hall London,1979.
2. J.O.M. Bockris and 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.
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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,* AddisonWesley.
3. K. Huary, *Statistical mechanics, Thermodynamics and Kinetics* , JohnWiley.
4. O.K.Rice, *Statistical mechanics, Thermodynamics and Kinetics,* Freeman andCo.
5. F.C. Andrews, *Equilibrium statistical mechanics* , John Wiley and sons,1963.
6. M.C. Guptha, *Statistical Thermodynamics* , Wiley eastern Ltd.,1993

M E S COLLEGE MAMPAD - AUTONOMOUS

M.Sc. CHEMISTRY – SEMESTER I & II

CHE1L01 & CHE2L04 – INORGANIC CHEMISTRY PRACTICALS– I & II

(3 Credits)

CHE1L01&CHE2L04	Inorganic chemistry practical I & Inorganic chemistry practical II*	P 4	C 3
Objectives	To develop the skill of identifying less common cations and quantitative determination of various metal ions.		
Course out comes	1.To enable the students to develop skill in the qualitative determination of common and less common cations from their mixture 2.To understand the theory of colorimetry and the way of determining the quantity of metal ions through this technique. 3. To enable the students to develop skill in the cerimetric determination of metal ions 4.To apply proper techniques for volumetric estimation of metal ions		

UNIT 1: Inorganic Cation MixtureAnalysis

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 ofwater)

(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 E S COLLEGE MAMPAD - AUTONOMOUS

M.Sc. CHEMISTRY – SEMESTER I & II

CHE1L02 & CHE2L05 – ORGANIC CHEMISTRY PRACTICALS– I & II

(3 Credits)

CHE1L02&CHE2L05	Organic chemistry Practical I & Organic chemistry Practical II*	P 4	C 3
Objectives	To develop the practical skills in separation of organic mixtures using simple acid -base chemistry,to determine the b.p&m.p of the compounds,to identify the functional groups present in the compound and to introduce different multistep synthesis to develop the skills in synthetic organic chemistry and strategic approaches for drug synthesis and analysis.		
Course out comes	1.Able to identify the functional groups present in the given organic compound		

	2.To learn the pilot separation of bi mixtures 3.To understand the techniques involving drying and recrystallisation of synthesised organic compounds by various methods and to determine their b.p&m.p 4.Able to synthesise solid derivatives of all organic compounds with different functional groups.		

Unit 1: Laboratory Techniques

Methods of Separation and Purification of Organic Compounds – fractional, steam and low-pressure distillations, fractional crystallisation 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 including green way of synthesis) and three stage (minimum two). Drawing the structure of organic molecules and reaction schemes by chemdraw,/ Symyx,/Chemsketch. Draw the structure and generate the IR and NMR spectra of substrates and products

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, Fuson andCartin, *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 OrganicChemistry*.
7. Pavia, Kriz, Lampman, and Engel, *A Microscale Approach to Organic Laboratory Techniques,* 5/e, Cengage,2013.
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M E S COLLEGE MAMPAD - AUTONOMOUS

M.Sc. CHEMISTRY – SEMESTER I & II

CHE1L03 & CHE2L06 – PHYSICAL CHEMISTRY – I &II (3 Credits)

CHE1L03&CHE2L06	Physical chemistry practical I & Physical chemistry practical II*	P 4	C 3
Objectives	Enable the students to design experiments to measure physical parameters of materials and understand the relation between physical property and chemical composition Introduce experiments related to the measurements of conductivity, refractive index, EMF , and construction of phase diagrams for two component systems. Introduce experiments related to thermochemistry and Nernst distribution law		
Course out comes	The students are expected to 1.Acquire analytical skills for measuring physical parameters 2.Understand the basic principle and applications of conductometric , potentiometric,refractometric and viscosity measurements 3.Acquire skills for handling instruments like conductivity meter ,potentiometer, refractometer etc 4. Construct phase diagram for two component systems 5.Calculate thermodynamic parameters from thermochemistry experimental data		

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 graphicalmethod

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 solidmixture.

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., polystyrenein

Unit 4: Distribution Law (minimum 3 experiments)

1. Determination of distribution coefficient of I_2 between CCl_4andH_2O.
2. Determination of equilibrium constant of KI + I_2 =KI_3
3. Determination of concentration of KIsolution

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 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_3-COOH) 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_3-COOH vsNaOH
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 pH meter

<u>Note.</u>

Students may be encouraged to plot graphs in graphing softwares like Sigma plot or Origin

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*, McGrawHill.
7. J. B. Yadav, *Advanced Practical Physical Chemistry*, *Goel Publications*,1989.
8. B. Viswanathan & R.S. Raghavan, *Practical Physical Chemistry,* Viva Books, 2009

M E S COLLEGE MAMPAD - AUTONOMOUS

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

CHE3C09 - MOLECULAR SPECTROSCOPY (4 Credits,72hrs)

CHE3C09	Molecular spectroscopy	L	C
		4	4
Objectives	Introduce and give adequate theoretical background of various spectroscopic techniques and enable the students to use various spectral data to characterise the materials		

Course out comes	The students are expected to 1. Understand the theoretical background of various spectroscopic techniques. 2. Understand the fundamentals of UV, IR, NMR and mass spectroscopy for the characterization of organic molecules. 3. Use combined spectral data of various techniques for the structural elucidation of organic compounds 4. Apply spectroscopic methods as analatytical tool for characterization of materials in chemistry, biology, and medicine and material science		

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

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* (9hrs)

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. **Introduction to FT-IR**

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, Ground and excited electronic states of diatomic molecules ,types of electronic transitions; Dissociation and pre-dissociation; Calculation of Dissociation energy-**Birge sponer method**. Electronic spectra of polyatomic molecules; Electronic spectra of conjugated molecules;

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

NMR: Quantum mechanical description of Energy levels-Population of energy-Transition probabilities -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* (9hrs)

Electron Spin Resonance: Quantum mechanical description of electron spin in a magnetic field- Energy levels-Population- Transition probabilities - 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.

Introduction to NQR

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

UV-Visible spectroscopy: Factors affecting the position and intensity of electronic absorption bands – conjugation, solvent polarity and steric parameters. Empirical rules for calculating $\lambda_{max}$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 and Axial 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 (9hrs)

^{1}HNMR: 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 (9hrs)

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

^{13}CNMR: 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 (9hrs)

Mass Spectrometry: Basic concept of EIMS. Molecular ion and meta stable 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, MALDI

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,—JohnWiley
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
7. William Kemp, Organic Spectroscopy**, 3e,** Palgrave,2010

M E S COLLEGE MAMPAD - AUTONOMOUS

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

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

CHE3C10	Organometallic And Bioinorganic chemistry	L	C
		3	4
Objectives	To understand the nature of metal-ligand bond,structure and bonding in metal carbonyls,nitrosyls,dinitrogen and dihydrogen compounds and the use of organometallic compounds in industrial catalysis. To learn about the effect of metal ion concentration and its physiological effects on various biological systems		
Course out comes	1.Acquire knowledge about the nature of ligands, its electron donating ability and bonding modes of ligands with metal ions. 2.Able to understand the stability and structural patterns of metal clusters,carbonyls and nitrosyls. 3.Able to identify the role of metal ions in the biological and physiological systems and applications.		

	4.Get knowledge about the homogeneous and heterogeneous organometallic catalysts in various industrial processes.		

Unit 1: Introduction to Organometallic Chemistry (9hrs)

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. Nytrosyl, dihydrogen and dinitrogen complexes. Transition metal to carbon multiple bond-metal carbenes and carbines.

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

Transition metal complexes with linear π- systems-Hapticity. Sythesis , 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 (9hrs)

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 (9hrs)

Metal-Metal bond and metal clusters. Bonding in metal-metal single,double,triple and quadruple bonded non-carbonyl clusters. Structure of $[Re_2X_8]^{2-}$. 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 (9hrs)

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 (9hrs)

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 B_{12} and coenzymes.Chlorophil II- Photosystem I and II. Nitrogen fixation-Nitrogenases.

Anticancer drugs, metals in medicine, therapeutic application of Cisplatin,radio isotope, MRI agents, toxic effect of some heavy metals

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, W*ileyEastern.

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 E S COLLEGE MAMPAD - AUTONOMOUS

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

CHE3C11- REAGENTS AND TRANSFORMATIONS IN ORGANIC CHEMISTRY

(4 Credits, 54hrs)

CHE3C11	Reagents and Transformations in Organic Chemistry	L 3	C 4
Objectives	To understand ; 1.various oxidants used for the oxidation of alcohols to carbonyl compounds 2.reducing agents 3.reactions and synthesis of heterocyclic compounds 4.reactions involving intermediates		
Course out comes	1.students are expected to understand the reagents used for oxidation and reductions 2.Students will be able to design the mechanisms of organic reactions. 3.students will acquire knowledge of supramolecular,polymer chemistry and type of interactions between molecules. 4.students will be able to identify selective reagents used for oxidation reactions		

Unit 1: Oxidations (9hrs)

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 CrO_3-Pyridine reagent. Oxidative cleavage of alkenes to carbonyls using O_3. Oxidative decarboxylation, Riley reaction, Baeyer-Villiger oxidation, Dess-Martin oxidation, Swern oxidation, hydroboration-oxidation.

Unit 2: Reductions (9hrs)

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 hrs)

Synthetic applications of Crown ethers, β-cyclodextrins, PTC, ionic liquids, Baker's yeast, NBS, LDA, $LiAlH_4$, $LiBH_4$, 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, DIBAL AIBN and Lindlar catalyst in organic synthesis

Unit 4: Chemistry of Polymers (9 hrs)

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 graftcopolymers.

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 hrs)

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 (9hrs)

Rearrangements occurring through carbocations, carbanions, carbenes and nitrenes such as Wagner-Meerwein, Demjanov, dienone-phenol, benzil- 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:

1. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press,2011.
2. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, 3/e, CRC Press,1998.
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.
8. V. K. Ahluwalia and R. Aggarwal, *Organic Synthesis: Special Techniques*, 2/e, Narosa Publishing House,2006.
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.
16. J.M.Lehn, *Supramolecular Chemistry*,VCH.

MES COLLEGE MAMPAD (AUTONOMOUS)

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

CHE3E01 - SYNTHETIC ORGANIC CHEMISTRY (ELECTIVE)

(4 Credits, 54hrs)

CHE3E01	Synthetic organic chemistry (Elective)	L	C
		3	4
Objectives	1. To enable students to acquire knowledge about various reagents used for organic synthesis. 2. To enable students to acquire knowledge on carbonyl compound chemistry. 3. To impart depth knowledge about palladium catalyzed coupling reactions including mechanism and synthetic application. 4. To impart knowledge on planning and designing of a synthetic route. 5. To develop knowledge on various heterocyclic compounds.		
Course out comes	1. Students acquire proper knowledge on various reagents used for organic synthesis. 2. Students can predict the products formed when different reagents are used in a reaction. 3. Students can evaluate the use of different reagents for various reactions. 4. Students acquire proper knowledge on carbonyl compounds. 5. Students understand the use and applications of different coupling reactions. 6. Students will be able to plan, design and expain the mechanism of synthesis of different organic compounds.		

	7. Students will be able to identify the synthons, synthetic equivalents, synthetic reagents and substrates required for a reaction leading to a particular product. 8. Students will acquire knowledge on synthesis, reactions and applications of heterocyclic compounds.		

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

Reagents for oxidation and reduction: Ozone, 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 (9hrs)

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 (9hrs)

Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides, amides. Substitution at □-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 sulfur ylides.Protecting groups, functional group equivalents, reversal of reactivity (Umpolung), Introduction to combinatorial chemistry.

Unit- 4. Coupling Reactions (9hrs)

Coupling Reactions: Palladium Catalysts 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 (9hrs)

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, uplong reactions and use in synthesis, Introduction to retrosynthetic analysis, Synthesis of longifolene, Corey lactone, Djerassi Prelog lactone

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

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 .

References:

1. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press,2011.
2. S. Warren and P. Wyatt, *Organic Synthesis: Strategy and Control*, JohnWiley
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., JohnWiley
7. MBSmithandJ.March:*AdvancedOrganicChemistry-Reactions,MechanismsandStructure,*

6th ed., John Wiley

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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 E S COLLEGE MAMPAD - AUTONOMOUS

M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV CHE4C12- INSTRUMENTAL METHODS OF ANALYSIS

(4 Credits, 72 hrs)

CHE4C12	Instrumental Methods of Analysis	L 4	C 4
Objectives	1.To introduce thermal,radiometric,electroanalytical optical methods 2. To understand principles of conventional procedures of analytical techniques. 3.To evaluate errors,deviations and variants 4.To provide knowledge of chromatographic procedures		
Course out comes	Students will be able to; 1.understand the principles of conventional procedures 2.Evaluate errors in measurements and to minimise errors while conduction of measurements.		

	3.Identify compounds from a mixture using chromatographic techniques. 4. Understand principle and procedures of optical amd electroanalytical methods.		

Unit 1: **Research Methodology (9hrs)**

Treatment of analytical data, accuracy and precision, 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

Introduction to Research methods- The search of Knowledge, Purpose of research, Scientific methods, role of theory, characteristics of research ,

Type of research-fundamental, historical, applied and experimental

Chemical Literature- Primary, secondary and tertiary source of literature. Classical and comprehensive , refrence literature.

Databases- Science Direct and chemical abstract.

scientific writing- research reports , thesis ,journal articles, books

Types of publication articles –communications, reviews, Bibliometric indicators

Unit 2: **Analytical chemistry (9hrs)**

Gravimetry: **s**olubility product and properties of precipitates-nucleation, growth and aging, co-precipitation and post precipitation, drying and ignition. Inorganic precipitating agents: NH_3, H_2S, H_2SO_4, $(NH_4)_2MoO_4$ and NH_4SCN.

Organic precipitating agents: oxine, cupron, cupferron, 1-nitroso-lnaphthol, dithiocarbamates, 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.

Food Analysis - crude protein, fat, crud fiber, carbohydrate, calcium, potassium, sodium, and phosphates in food , food adulteration – common adulterats examination of foods for adulterants, Pesticide analysis in food products.

Forensic analysis- Analysis of Poisonous elements like As, Sb, Pb, Cr and Hg. Anaysis of – Insecticides, metals, gun powder residues, cyanides, dioxines & asbestos.

Analysis of biological fluids-Estimation of Hb, Urea and Creatinine

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

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 asbiosensors, 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 (9hrs)

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.

Unit5 Optical Methods - I (9hrs)

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 hrs)

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

Unit 7: **Thermal and Radiochemical Methods (9hrs)**

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 hrs)

Chromatography-classification-column-paper and thin layer chromatography. HPLC-outline study of instrument modules. Ion – exchange chromatography-Theory. Important applications of chromatographic techniques. Gel PermeationChromatography.

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 byGC

References:

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

02. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Fundamentals of AnalyticalChemistry,* 9th Edn., Cengage Learning., 2014.

03. J.G. Dick, *Analytical Chemistry*, R.E. KriegerPub.,1978.50

04. J.H. Kennedy, *Analytical Chemistry: Principles*, Saunders College Pub.,1990.

05. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, *Vogel's Text Book of Quantitative Chemical Analysis*, 5th Edn., John Wiley&sons,1989.

06. C.L. Wilson, D.W. Wilson, *Comprehensive Analytical Chemistry*, Elsevier,1982.

08. G.D. Christian, J.E. O'Reilly, *Instrumental Analysis*, Allyn & Bacon,1986.

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

10. A.I. Vogel, *A Textbook of Practical Organic Chemistry*, 5/e Pearson,1989.

11. H.A. Laitinen, W.E. Harris, *Chemical Analysis,* McGrawHill,1975.

12. V.K. Ahluwalia, *Green Chemistry: Environmentally Benign Reactions*, CRC,2008.

13. F.W. Fifield, D. Kealey, *Principles and Practice of Analytical Chemistry,* Blackwell Science,2000.

14. G.Gringauz, *Introduction to Medical Chemistry,* Wiley-VCH,1997.

15. Harkishan Singh and V.K.Kapoor, *Medicinal and Pharmaceutical Chemistry,* Vallabh Prakashan,2008.

16. W.Bannwarth and B.Hinzen, *Combinatorial Chemistry-From Theory to Application,2nd*

Edition, Wiley-VCH, 2006.

17. A.W.Czarnik and S.H.DeWitt, *A Practical Guide to Combinatorial Chemistry,* 1st Edition, American Chemical Society,1997.

18. Bansal N K, Kleeman M and Mells M, *Renewable Energy Sources and Conversion Technology,* Tata McGraw-Hill.(1990)

19. Kothari D.P., *"Renewable energy resources and emerging technologies",* Prentice Hall of India Pvt. Ltd.,2008.

20. Rai G.D, *"Non-Conventional energy Sources",* Khanna Publishers,2000.

21. Michael Grätzel, *J. Photochemistry and Photobiology C: Photochemistry Reviews* 4 (2003) 145–153, *Solar Energy Conversion by Dye-Sensitized Photovoltaic Cells*, Inorg. Chem., Vol. 44, No. 20, 20056841-6851.

M E S COLLEGE MAMPAD - AUTONOMOUS

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

CHE4E06 - NATURAL PRODUCTS & POLYMER CHEMISTRY (4 Credits, 72 hrs)

CHE4E06	Natural Products & Polymers (Elective)	L	C
		4	4
Objectives	1.To introduce the students in the field of natural products and their classifications. 2. To provide the students a broad idea about terpenoids, steroids, alkaloids ,and anthocyanins and their occurrence, structure, biosynthesis and properties. 3.The students will be familiar with the different dyes and pigment 4.To gain detailed knowledge about different types of polymerization processes, various mechanisms and Characterization processes. 5.Understanding a detailed idea about industrial polymers , copolymers, and optoelectronic properties of polymers.		
Course out comes	1.Acquire knowledge of the classification of the natural products by their molecular structures and biosynthesis. 2.Aqcuire knowledge of the functions of important natural products and the methodology used in natural product chemistry 4.Get a comprehensive knowledge about different polymerization techniques and characterizations. 5.Can interpret the stereochemistry of polymers and the knowledge of optoelectronic properties of polymers and their application in to electronic research		

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

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 ofimportant 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 hrs)

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 andsteroids.

Steroids:Classification and structure elucidation of Cholesterol, Ergosterol, Oesterone,Androsterone, Testosterone, Progestrone, Cortisone and Corticosterone.

UNIT 3: Alkaloids and Anthocyanins (9 hrs)

Alkaloids – classification of alkaloids, structure elucidation based on degradative reactions (quinine and atropine). Biosynthesis of quinine andpapaverine.

Anthocyanins**:** Introduction, General Nature and Structure of Anthocyanidins. Flavone, Flavonol, Isoflavone and Chalcone

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

Brief introduction to dyes and pigments (natural and synthetic): □-carotene, indigo, cyclic tetrapyrroles (porphyrins, chlorins, chlorophyll, heme), study of phthalocyanines, squarenes, 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., PlenumPress.
3. T.W. G. Solomons: *Fundamentals of Organic Chemistry*, 5th ed., JohnWiley
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, OxfordUniversityPress
8. N. R. Krishnaswamy: *Chemistry of Natural Products*; A Unified Approach, UniversitiesPress

9. R. J. Simmonds: *Chemistry of Biomolecules: An Introduction*,RSC

10. R. O. C. Norman: *Principles of Organic Synthesis*, 3rd ed., CRC Press,1998.

11. J. M. Lehn, *SupramolecularChemistry*

UNIT 5: Polymerization Processes (9 hrs)

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 dispersiontechniques

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

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 oxidecatalysts.

Polymer Characterization. Molecular weights. Concept of average molecular weights, Molecular weight distribution. Methods for determining molecular weights from colligative properties and viscocity measurements . 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-raydiffraction,

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

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 betweencrosslinks.

Industrial polymers. Synthesis, Structure and applications. Polyethylene, polypropylene, polystyrene.

Homo and Copolymers. Diene rubbers. Vinyl and acrylic polymers. PVC, PVA, PAN, PA. PMMA and relatedpolymers.

Copolymers. EVA polymers. Flourine containing polymers. Polyacetals. Reaction polymers. Polyamides, polyesters. Epoxides, polyurethanes, polycarbonates, phenolics, PEEK, Silicone polymers.

UNIT 8: Speciality Polymers (9 hrs)

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, 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 EasternLtd.
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 E S COLLEGE MAMPAD - AUTONOMOUS

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

(4 credits, 72hrs)

CHE4E08	Organometallic Chemistry	L	C

		4	4
Objectives	The learners should be able to analyze the mechanism of selected catalytic organic reactions from the structure-bonding aspects and reactivity of simple organometallic compounds. To know and understand the different properties and structures for organometallic compounds from different parts of the periodic table,principal synthetic routes to various classes of organometallic compounds. To know and understand the reactivity of organometallic compounds including their application in synthesis and catalysis		
Course out comes	1.Able to identify the structure and bonding aspects of simple organometallic compounds. 2.Apply different electron counting rules to predict the shape/geometry of low and high nuclearity metal carbonyl clusters 3.Identify the different types of organometallic reactions and apply the above concepts to explain different catalytic reactions. 4..Able to understand fundamental reaction types and mechanisms and how to combine these to understand efficient catalytic processes in small scale and large scale by homogeneously/heterogeneously		

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, H_2, 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 H_2, N_2, O_2, 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. SN^2 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 E S COLLEGE MAMPAD - AUTONOMOUS

M.Sc. CHEMISTRY – SEMESTER III & IV

CHE3L07 & CHE4L10 – INORGANIC CHEMISTRY PRACTICALS– III & IV

(3 Credits)

CHE3L07& CHE4L10	Inorganic chemistry practical III & Inorganic chemistry practical IV	P 4	C 3
Objectives	To make the student conversant with volumetric,gravimetric and colorimetric estimation of ions in a binary mixture and preparation of inorganic complexes.		
Course out comes	The students will be able to 1. Quantitatively separate and estimate ions in a binary mixture using volumetric,gravimetric and colorimetric techniques. 2.Understand solvent extraction technique. 3.Expertise in Ion- exchange separation and estimation of binary mixtures 4.Prepare inorganic complexes.		

Unit 1: Estimation of ions in mixture

Estimation involving quantitative separation of suitable binary mixtures of ions in solution (Cu^{2+}, Nl^{2+}, Zn^{2+}, Fe^{3+}, Ca^{2+}, Mg^{2+}, Ba^{2+} and Cr_2O1^{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 InorganicChemistry*.

M E S COLLEGE MAMPAD - AUTONOMOUS

M.Sc. CHEMISTRY – SEMESTER III & IV

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

CHE3L08& CHE4L11	Organic chemistry Practical III & Organic chemistry Practical IV	P 4	C 3
Objectives	1. To develop estimation skill of different organic compounds volumetrically. 2. To develop estimation skill of different organic compounds by colorimetric method. 3. To develop the skill of separation and identification of different organic compounds by chromatographic techniques.		
Course out comes	1. Students develop skill in the estimation of reducing sugar, amino group, phenolic group and esters volumetrically. 2. Students develop skill in the estimation of vitamin C, drugs and anti-biotics colorimetrically. 3. Students develop skill in the estimation the extraction of natural products and purification by column chromatography and TLC 4. Students develop skill in the prepartion of chromatographic plate and chromatographic paper for the separation and identification of various organic compounds. 5. Students develop skill in theTLC plate activation and identification of compoundsdyes, food additives, food colours, amino acids, sugars, pesticides and herbicides		

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, *PharmacueticalAnalysis*.

Unit 2: Extractions

Extraction of Natural products and purification by column chromatography and TLC – Caffeine from Tea waste, Chlorophill 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, Benzalacetate, 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 OrganicChemistry*.

M E S COLLEGE MAMPAD - AUTONOMOUS

M.Sc. CHEMISTRY – SEMESTER III & IV

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

CHE3L09& CHE4L12	Physical chemistry practical III & Physical chemistry practical IV	P 4	C 3
Objectives	Introduce and design experiments for measurements for kinetic parameters of ester hydrolysis ,adsorption,three component system, miscibility etc . Introduce and familiarize computational chemistry programmes like Gaussian /firefly and enable students to apply those programmes to the problems in chemistry		
Course out comes	The students are expected to 1.Verify experimentally the fundamental concepts related to kinetics 2.Understand, apply and verify various adsorption isotherms related to adsorption from solution 3. Construct phase diagram for three components systems 4. Familaralize computational chemistry programme firefly and apply the programmes for the calculation of energy ,prediction of geometry,frequency etc		

SECTION A

Unit 1: Chemical Kinetics (4experiments)

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 ethylacetate or methyl 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-acetic acid system. Determination of the concentration of a given acetic acid solution using the isotherm

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

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 li quid 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 solutionof

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 ofNaCl.

4. Study of the reaction 2Kl + Hgl 2 .K_2Hgl_4 and determination of the concentration of the given Klsolution.

Unit 5: Polarimetry (3 experiments)

1. Determination of specific and molar optical rotations of glucose, fructose andsucrose.
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 H_2O and NH_3 at the HF/3-21G level of theory.
2. The effect of basis set on the single point energy of H_2O and NH_3 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 H_2O, NH_3, HCHO & C_2H_4 at the HF/6-31G level of theory.
4. Computation of dipole and quadrupole moments of HCHO& C_2H_4 at the HF/6-31G level of theory.
5. Effect of basis set on the computation of H-O-H bond angle in H_2Ousing 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 ethyleneat the HF/6-31G level of theory.
7. Effect of substituent (F & Cl) on the geometric parameters (like C-C bond length) of ethyleneat the HF/6-31G level of theory.
8. Comparison of stability of cis-planar and trans-planar conformers of H_2O_2at the HF/6-31G level of theory.
9. Comparison of stability of cis- and trans- isomers of difluoroethyleneat the HF/6-31G* level of theory.
10. Computation of the frequencies of normal modes of vibration of molecules likeH_2O, NH_3 and CO_2at the HF/6-31+G* level of theory.
11. Determination of hydrogen bond strength of H_2O dimer and H_2O trimer at the HF/6-31+G* level of theory.
12. Dete+rmination 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

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