ST. JOSEPH'S COLLEGE (AUTONOMOUS), DEVAGIRI, CALICUT

Syllabus
for

M.Sc. CHEMISTRY PROGRAMME

Under

CHOICE BASED CREDIT SEMESTER SYSTEM-PG-2019

(With effect from 2019 admission onwards)

ST. JOSEPH'S COLLEGE (AUTONOMOUS)
DEVAGIRI,CALICUT

M.Sc. CHEMISTRY (CBCSS PATTERN)

Regulations and Syllabus with effect from 2019 admission

The Board of Studies in Chemistry at its meeting held on 28-01-2019 considered the revision of M.Sc. Chemistry syllabus under Credit Semester System (CBCSS) 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 at its meeting held on 07-06-2019 are given below:

The pattern of the Programme

a) The name of the programme shall be **M.Sc. Chemistry under CBCSS 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 are given in Table 1. The programme shall be conducted in accordance with the programme pattern, the scheme of examination and syllabus prescribed. Of the 25 hours per week, 13 hours shall be allotted for theory and 12 hours for practicals. 1 theory hour per week during III and IVsemesters 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. College 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. College 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 core theory courses in the second 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 the second and fourth semesters. At the end of the second semester, three practical examinations with the codes FCHE2L01, FCHE2L02, & FCHE2L03 will be conducted. Practical examinations for the codes FCHE4L04 & FCHE4L05, & FCHE4L06 will be conducted at the end of the fourth semester. **Each practical examination will be of six-hour duration with 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 recognized 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 the reputed industry can be considered. Each student has to submit three copies of the project dissertation for valuation at the end of the 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 the fourth semester, after the theory examinations. Viva-voce on the project will also be conducted on the same day.

A comprehensive viva voce examination (2 credits), 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 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.**

(3) 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.

(4) Evaluation and Grading should be done by the direct grading system. Evaluations of answers are done on a 6-point scale (A+, A, B, C, D, E). Grades and grade points are given as shown 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 a 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 will be 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

(5) 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(or 20%)
External	4 (or 80%)

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

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

Theory: 5 weightages

(a) Internal Examinations- weightage = 2 (2 internal exams, both should be considered)
(b) Assignments and Exercises- weightage = 1
i. Seminars/Viva Voce- weightage = 1
ii. Attendance –weightage = 1

Corresponding to the WGPA obtained in internal test papers grades and grade points can be assigned as given below for the purpose of computing internal marks.

WGPA	Grade	Grade point
4 to 5	A+	5
3 to >4	A	4
2 to >3	B	3
1 to >2	C	2
>1	D	1

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

Practical: 10 weightages

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 examsis considered)
d) Record-weightage = 2
e) Viva Voce- weightage = 2

Project: 10 weightages

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 the 4th semester).

(7) External evaluation:

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

The 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 question paper				**30**

b) **Practicals**: At the end of II and IV semesters, there will be three practical examinations. 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 of 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) Significance 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 the project is 4.

(8) Directions for question papersetters:
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.
(Further details regarding the grading and evaluation are as per the PG regulations 2019)

Dr. Joy Joseph
Chairman, Board of Studies in Chemistry,
St. Joseph's College (Autonomous) Devagiri, Calicut

Audit courses:

Ability Enhancement Course (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 an audit credit course and should be conducted during the first semester of the programme. The credit of the AEC 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 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. 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
AEC, which will be decided by the department council/ HoD.

a) Industrial/Research institution visit/visits

b) Publication of a research article/articles in the 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 are presented in a national level seminar/conference and published in the proceedings

e) Internships at any reputed research institutions/R&D centre/Industry

f) Submission and presentation of a review article on a research work which won Nobel Prize in Chemistry after 2000.

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 controller 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 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, Gamess etc 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 controller 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 controller. 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 CBCSS Patten (2019 onwards)

Semester	Course Code	Course Title	Instruction /week	Credits
1	FCHE1C01	Quantum Mechanics and Computational Chemistry	4	4
	FCHE1C02	Elementary inorganic chemistry	3	4
	FCHE1C03	Structure and reactivity of organic Compounds	3	4
	FCHE1C04	Thermodynamics, kinetics, and catalysis	3	4
	FCHE1A01	Ability Enhancement Course (AEC)		4*
	FCHE2L01	Inorganic chemistry practical I	4	Examinationat the end of second semester
	FCHE2L02	Organic chemistry Practical I	4	
	FCHE2L03	Physical chemistry practical I	4	
		Total Credits	**Core**	**16**
II	FCHE2C05	Group theory and Chemical Bonding	3	3
	FCHE2C06	Coordination chemistry	3	3
	FCHE2C07	Reaction Mechanism in Organic Chemistry	3	3
	FCHE2C08	Molecular spectroscopy	4	3
	FCHE2A02	Professional Competency Course (PCC)		4*
	FCHE2L01	Inorganic Chemistry practical I	4	3
	FCHE2L02	Organic Chemistry Practical I	4	3
	FCHE2L03	Physical Chemistry practical I	4	3
		Total Credits	**Core**	**21**
III	FCHE3C09	Electrochemistry, Solid stateChemistry, and Statistical Thermodynamics	3	4
	FCHE3C010	Organometallic &Bioinorganic Chemistry	3	4
	FCHE3C011	Photochemistry and Pericyclic Reactions	3	4
	FCHE4L04	Inorganic Chemistry practical II	4	Examinationat the end of fourth semester
	FCHE4L05	Organic Chemistry Practical II	4	
	FCHE4L06	Physical Chemistry practical II	4	
	FCHE3E01	Synthetic organic chemistry (Elective)	3	4
	FCHE3E02	Computational Chemistry (Elective)	3	4
	FCHE3E03	Industrial Catalysis (Elective)	3	4
		Total Credits	**Core** **Elective**	**12** **4**

Semester	Course Code	Course Title	Instruction /week	Credits
IV	FCHE4C12	Instrumental Methods of Analysis	4	4
	FCHE4L04	Inorganic Chemistry Practical II	3	3
	FCHE4L05	Organic Chemistry Practical II	3	3
	FCHE4L06	Physical Chemistry Practical II	3	3
	FCHE4E04	Petrochemicals and Cosmetics (Elective)	4	4
	FCHE4E05	Supra-molecular, Medicinal and Green Chemistry (Elective)	4	4
	FCHE4E06	Natural products & Polymer Chemistry (Elective)	4	4
	FCHE4E07	Material Science (Elective)	4	4
	FCHE4E08	Organometallic Chemistry(Elective)	4	4
	FCHE4P01	Research Project	3	4
	FCHE4V01	Viva Voce		2
		Total Credits:	**Core** **Elective** **Project** **Viva**	**13** **8** **4** **2**
	TOTAL CREDITS OF THE PROGRAMME : **CORE** **ELECTIVE** **PROJECT** **VIVA-VOCE** ***TOTAL CREDITS***			 **62** **12** **4** **2** **80**

* The credit of the AEC/PCC will not be considered while calculating the SGPA/CGPA

Programme Specific Outcome

PSOs	PROGRAMME SPECIFIC OUTCOMES
PSO1	Understand basic concepts in chemistry and apply the basic theoretical principles of chemistry
PSO2	To appreciate the achievements in chemistry and to know the role of chemistry in nature and in society
PSO3	Generate awareness on the emerging areas of chemistry, their applications and to appraise the students of its relevance in future studies
PSO4	To develop skills in the proper and safe handling of instruments and chemicals
PSO5	To familiarize with the different processes used in industries and their applications
PSO6	To develop an eco-friendly attitude by creating a sense of environmental awareness and importance of green chemistry
PSO7	Create interest in research in various fields of chemistry through research project work and seminars
PSO8	Competency to clear various entrance examination for higher study such as CSIR-UGC, NET (LS), SET, PSC exams
PSO9	Develop the spirit of team work and effective communication skill
PSO10	Awareness about future challenges before the scientific community and enable them to face these challenges through systematic planning and hard work

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

FCHE1C01: QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(4 Credits, 72 hours)

COs	COURSE OUTCOMES
CO1	To categorize translational, rotational, vibrational motion of molecules quantum mechanically
CO2	To evaluate the importance of approximation methods to solve systems of many electrons
CO3	To summarize the different methods used in computational chemistry
CO4	To gain an insight into the structure of Gaussian file and how it is applied to find molecular parameters

Unit 1: Introduction to Quantum Mechanics (9hrs)

Black body radiation and Planck’s quantum postulate. Einstein’s photoelectric equation, Schrodinger’s wave mechanics, Detailed discussion of postulates of quantum mechanics – State function or wave function postulate, Born interpretation of the wave function, well behaved functions, orthonormalityof 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, Symmetrybreaking.

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.Ladder operators.

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. Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta ((L_x, L_y, L_z), commutation relations between these 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. The postulate of spin by Uhlenbeck and Goudsmith, Dirac's relativistic equation for hydrogen atom and discovery of spin (qualitative treatment), spin orbitals, construction of spin orbitals from orbitals and 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 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 (9 hrs)

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

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

Electronic structure of molecules – Basics of HF-SCF method of molecules (derivation not required). 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), Concept of electron correlation and post HF methods. (Elementary idea)

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 andb) Internal coordinates. The Z-matrix - Z- matrices of some simple molecules like H_2,H_2O, formaldehyde ammonia and methanol.

Reference (for units 1 to 6)

1. F.L. Pilar, *Elementary Quantum Chemistry* , McGraw-Hill,1968.
2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson EducationInc.,
3. P.W.AtkinsandR.S.Friedman,*MolecularQuantumMechanics*,4th Edition,OxfordUniversity 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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10. L. Pauling and E.B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1935 (A good source book for many derivations).
11. R.L. Flurry, Jr., *Quantum Chemistry*, Prentice Hall,1983.
12. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International,2006.
13. M.S. Pathania, *Quantum Chemistry and Spectroscopy (Problems & Solutions)*, Vishal Publications,1984.
14. C.N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry*, Prism Books Pvt. Ltd.,1998.
15. Jack Simons, *An Introduction to Theoretical Chemistry*, Cambridge University Press, 2003.

Reference (for units 7 & 8)

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

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

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

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

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

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

FCHE1C02 - ELEMENTARY INORGANIC CHEMISTRY

(4 Credits, 54 hrs)

COs	**COURSE OUTCOMES**
CO1	To differentiate between different acid-base concepts.
CO2	To discuss the chemistry of main group, transition and inner transition elements.
CO3	To predict the stability of nuclei.
CO4	To explain the importance of Nano materials.

Unit 1: Molecular Structure and Bonding (9hrs)

The Lewis structure – Octet rule- Resonance – Formal charge –hyper valence electro neutrality principle- Iso electronic molecules. VSEPR theory, Walsh diagrams, dπ – pπ bonds. Bent rule and energetics of hybridization. The hydrogen bond and its consequences-van der Waal`s forces-Determination of molecular structure by X-Ray diffraction.

Unit 2: 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 HSAB concept. Chemistry of non aqueous solvents- NH_3, SO_2, H_2SO_4, BrF_3, HF, N_2O_4 and HSO_3 F. Non aqueous solvents and acid-base strength. Super acids –surfaceacidity.

Unit 3: Chemistry of Main Group Elements-I (9hrs)

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

Unit 4: 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 5: 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, Uranyl compounds. Trans-actinide elements. Super heavy elements –production and chemistry.

Unit 6: 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 radiation dosimetry.

References

1. N.N.GreenwoodandA.Earnshaw,*ChemistryofElements,2/e,Elsevier*Butterworth-Heinemann,2005.
2. J.E.Huheey,E.A.Keiter,R.L.Keiter.O.K.Medhi.*InorganicChemistry,principlesof 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. WilliamWPorterfield,*InorganicChemistry-Aunifiedapproach,*Academic Press,2005.
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M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I
FCHE1C03: STRUCTURE AND REACTIVITY OFORGANIC COMPOUNDS
(4 Credits, 54 hrs)

COs	COURSE OUTCOMES
CO1	To predict and demonstrate the aromaticity of organic compounds.
CO2	To analyse the effect of conformation on the rate of reactions.
CO3	To categorize different types of stereoisomerism in organic compounds.
CO4	To summarize the basic aspects of asymmetric synthesis.

Unit 1. Aromaticity and Reactions (9 h)

Aromaticity: Qualitative application of Huckel MO theory and perturbation theory (PMO approach) to systems containing delocalized electrons. Concept of aromaticity, delocalization of electrons – Huckel’s rule, criteria for aromaticity, examples of neutral and charged aromatic systems – annulenes – anti- and homo- aromatic systems. Aromaticity of fulvenes, fulvalenes, azulenes, pentalenesand heptalenes.

Aromatic Electrophilic Substitution: Arenium ion mechanism, orientation and reactivity (ortho, meta and para directing groups), ortho/para ratio, ipso attack. Typical reactions – Diazonium coupling, Vilsmeier-Haack reaction, Gattermann-Koch reaction, Pechman reaction and Houben-Hoesch reaction.

Aromatic Nucleophilic Substitution: Addition-elimination (S_NAr), elimination-addition (benzyne), S_N1 (reaction of diazonium salts without copper salts) and $S_{RN}1$ (reaction of diazonium salts with copper salts) mechanisms.

Unit 2. Reaction Mechanism: Structure and Reactivity (9 h)

Types of reaction, types of mechanisms, thermodynamic and kinetic requirement, kinetic and thermodynamic control, Hammond’s postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, kinetic isotope effects, methods of determining mechanisms.

Effect of structure on reactivity – resonance and field effects, steric effect, quantitative treatment. Linear free energy relationships, Hammet and Taft equations, □ and □ parameters; Applications of acid-base concept-HSAB theory.

Unit 3: Conformational Analysis – I (9 h)

Difference between configuration and conformation. Internal factors affecting the stability of molecules – dipole interaction, bond opposition strain, bond angle strain. Conformational analysis of acyclic compounds: ethane, propane, *n*-butane alkene dihalides, glycols, chlorohydrins, tartaric acid, erythro and threoisomer.

Conformations of carboxylic rings of different sizes three to seven. Conformations ofmonosubstitutedcyclocyclohexanes (monomethyl, *iso*-propyl, *tert*-butyl and di-substituted cyclohexanes (dialkyl, dihalo, diols). Anchoring group and conformationaly biased molecules. Conformations of fused, bridged and caged ring systems-decalins, norbornane, barrelene, and adamantanes. Conformational analysis of glucose, ribose and galactose. The role of anomeric effect in the conformation of cyclic compounds. Chemical consequence of conformational equilibrium – Curtin Hammett principle.

Unit 4: Conformational Analysis – II (9 h):

Effect of conformation on the course and rate of reactions: (a) Debromination of vicinal dibromides using KI, (b) Semipinacolic deamination of α-amino alcohols, (c) Dehydrohalogination of vicinal dihalides. Effect of conformation on the course and rate of reactions in cyclohexane systems illustrated by: (a) S_N2 and S_N1 reactions for (i) an axial substituent, and (ii) an equatorial substituent in flexible and rigid systems. (b) E1, E2 eliminations in substituted halocyclohexanes and cyclohexyltosylate. (c) Pyrolytic elimination of cyclohexyl esters. (d) Compare the rate of esterification of methanol, isomenthol, neomenthol and neoisomenthol (e) Oxidation of secondary axial and equatorial hydroxyl group to ketones by chromic acid.Conformational analysis and trans-annular reactions of medium rings: Hydrolysis of epoxides and bromination of C_8 – C_{10} cyclic dienes. Polar substituent effects in the reduction of cyclohexanones and norbornan-7-ones. Percent axial and equatorial approach in reduction of 2-substituted 4-*t*- butyl cyclohexanones.

Unit 5. Stereochemistry (9 h)

Stereoisomerism: Fischer, Newman and Sawhorse projection formulae and their inter conversion. Molecular symmetry and chirality. Molecules with C, N, S based chiral centers - absolute configuration, enantiomers, racemic modifications, diastereoisomers. Axial, planar and helical chirality with examples. R and S nomenclature using Cahn-Ingold-Prelog rules.

Optical purity, enantiomeric excess and diastereomeric excess and their determination. Racemisation and resolution: Mechanism of racemisation - Methods of resolution: Preferential cystallization, kinetic resolution, chiral chromatography, biochemical methods and through inclusion compounds.

Geometrical isomerism – E and Z notation of compounds with one and more double bonds in acyclic systems. Configuration of cyclic compounds- monocyclic, fused and bridged ring systems, interconversion of geometrical isomers. Methods of determination of the configuration of geometrical isomers. Optical activity in *cis-trans* conformational isomers of 1,2-, 1,3- and 1,4-dimethylcyclohexanes.

Topicity and prostereoisomerism, prochiral centre, enantiotopic, homotopic, diastereotopic hydrogen atoms, topicity of ligands and faces as well as their nomenclature-Pro-R, Pro-S, Re and Si.

Stereoselective and stereospecific reactions: (i) Bromination of *E*-and *Z*-2-butene-a stereospecific *anti* addition, (ii) Epoxidation of E-and Z-2 butene-a stereospecific reaction, (iii) Bromination of cyclohexene- a stereoselective reaction, (iv) Hydroboration-Oxidation hydration of alkenes- a stereospecific *anti*-markovnikov hydration (v) Addition of carbenes to alkenes.

Unit 6: Asymmetric Synthesis (9 h)

Asymmetric synthesis, need for asymmetric synthesis, stereoselectivity and stereospecificity.

Strategies in Asymmetric Synthesis:

Chiral pool: Amino acids in the synthesis of benzodiazepines- conversion of L-tyrosine into L-Dopa; synthesis of beetle pheromone component (*S*)- (–)-ipsenol from (S)-(–)-leucine, Carbohydrates – (*R*) Sulcatol from 2-deoxy-D-ribose.
Substrate controlled: Nucleophilic additions to chiral carbonyl compounds. 1,2- asymmetric induction, Cram's rule, Crams chelation control, Prelog's rule and Felkin-Anh model. Diastereofacial Selectivity in the Aldol Addition Reaction - Zimmerman-Traxler model.
Chiral auxiliary controlled: Oxazolidinone controlled Diels-Alder reaction and α-alkylation of chiral enolates. Enantioselective aldol condensation via chiral enolates
Chiral reagent controlled: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2BH and $IPCBH_2$. Reduction with CBH reagent. Sharpless asymmetric epoxidations and dihydroxylation.
Chiral catalyst controlled: Rhodium and Ruthenium catalysts with chiral phosphine ligands

like BINAP and DIOP. Preparation and use of CBS asymmetric reducing agent, baker's yeast reduction.

References:

1. F.A. Carey, R.A. Sundberg, *Advanced Organic Chemistry, Part A and B: Structure and Mechanisms*, 5/e, Springer, 2007.
2. M. B. Smith, J. March, *March's Advanced Organic Chemistry*, John Wiley & Sons, 6/e, 2007.
3. R. Bruckner, *Advanced Organic Chemistry: Reaction Mechanisms*, Academic Press, 2002.
4. J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press, 2004.
5. T.H. Lowry, K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, 2/e, Harper & Row, 1981.
6. E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books, 2005.
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8. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*, 3/e, New Age Pub., 2010.
9. P. S. Kalsi, *Stereochemistry*, 4/e, New Age International Ltd.
10. P.S. Kalsi, *Organic reactions & their mechanisms*, 3/e revised, New Age International Ltd.
11. G. L. D. Krupadanam, *Fundamentals of Asymmetric Synthesis*, Universities Press, 2013.

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

FCHE1C04 – THERMODYNAMICS, KINETICS AND CATALYSIS

(4 Credits, 54 hrs)

COs	**COURSE OUTCOMES**
CO1	To compare and contrast the principles of reversible and irreversible thermodynamics.
CO2	To apply the basic concepts of chemical kinetics to study rates of different types of reactions.
CO3	To categorize the different theories of reaction rates.
CO4	To apply the basics of adsorption to determine surface parameters.
CO5	To analyse the different theories of catalysis.

Unit 1: Thermodynamics (9 hrs)

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

Unit 6: Catalysis (9 hrs)

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:

1. P. Atkins & J. De Paula, *Atkins's Physical Chemistry, 10/e, OUP, 2014*.
2. Keith J. Laidler, *Chemical Kinetics 3rd edn.*, Pearson Education, 1987(Indian reprint 2008).
3. Steinfeld, Francisco and Hase, *Chemical Kinetics and Dynamics, 2ndedition,*Prentice Hall International . Inc

4. Santhosh K. Upadhyay, *Chemical Kinetics and Reaction Dynamics,* Springer,2006.

5. Richard I. Masel, *Chemical Kinetics and Catalysis* , Wiley Interscience,2001.

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11. Rajaram and Kuriokose, *Thermodynamics,* East-West1986

12. Prigoggine, *An Introduction to Thermodynamics of Irreversible Processes*, Interscience

13. B.G. Kyle, *Chemical and Process Thermodynamics*, 2nd Edn, Prentice Hall ofIndia

14. A. W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces,* 6 Edn.,Wiley,2011.

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

16. Dipak Kumar Chakrabarty, *Adsorption and Catalysis by Solids*, New Age.2007.

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

18. Woodruff, D. P. and Delchar T. A., *Modern Techniques of Surface Science*, Cambridge Solid State Science Series, 1994.

19. Kurt K. Kolasinski, *Surface Science: Foundations of Catalysis and Nanoscience,* 3^{rd}Edn., Wiley U. K.,2012.

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

FCHE2C05 - GROUP THEORY AND CHEMICAL BONDING

(3 Credits, 54hrs)

COs	COURSE OUTCOMES
CO1	To correlate the principles of Group theory and quantum mechanics.
CO2	To apply the principles of group theory for spectroscopic analysis.
CO3	To apply the principles of group theory to study chemical bonding in diatomic and polyatomic molecules.
CO4	To describe the chemical bonding in diatomic and 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 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 ofsymmetry operations of a molecule, point groups and their systematic identification, GMTofpointgroups;

Mathematical preliminaries - matrix algebra, addition and multiplication of matrices, inverse of a matrix, square matrix, character of a square matrix, diagonal matrix, direct product and direct sum of square matrices, block factored matrices, solving linear equations by the method of matrices;

Matrix representation of symmetry operations.

UNIT 2: Representations of Point Groups & Corresponding Theorems (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., Γ_{cart}) using the reduction formula;

Relation between group theory and quantum mechanics – wavefunctions (orbitals) as bases for IR of point groups.

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

Molecular vibrations - symmetry species of normal modes of vibration, construction of

Γcart, normal coordinates and drawings of normal modes (e.g., H_2O and NH_3), selection rules for IR and Raman activities based on symmetry arguments, determination of IR active and Raman active modes of molecules (e.g., H_2O, NH_3, CH_4 , SF_6), complementary character of IR and Raman spectra.

Spectral transition probabilities - direct product of irreducible representations and its use in identifying vanishing and non–vanishing integrals, transition moment integral and spectral transition probabilities.

Electronic Spectra – electronic transitions and selection rules, Laporte selection rule for centro symmetric molecules.

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

Hybridisation - Treatment of hybridization in BF_3 and CH_4, Inverse transformation and construction of hybrid orbitals. Molecular orbital theory – HCHO andH_2O as examples, classification of atomic orbitals involved into symmetry species, group orbitals, symmetry adapted linear combinations (SALC), projection operator, construction of SALC using projection operator, use of projection operator in constructing SALCs for the MOs in cyclopropenyl ($C_3H_3^+$)cation.

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 bondorders from the coefficients of HMO, calculation of free valence, HMO theory of aromatic hydrocarbons (benzene); formula for the roots of the Hückel determinantal equation, Frost -Hückel circle mnemonic device for cyclic polyenes.

Reference (for Units 1 to 4)

1. F.A. Cotton, *Chemical applications of Group Theory*, 3rdEdition, John Wiley &Sons Inc.,2003.
2. H. H. Jaffe and M. Orchin, *Symmetry in Chemistry,* John Wiley &Sons Inc.,1965.
3. L.H. Hall, *Group Theory and Symmetry in Chemistry*, McGraw Hill,1969.
4. R. McWeeny, *Symmetry: An Introduction to Group Theory and its Applications*, Pergamon Press, London,1963.
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6. Mark Ladd, *Symmetry & Group Theory in Chemistry*, Horwood1998.
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10. A.W. Joshi, *Elements of Group Theory for Physicists,* New Age International Publishers,1997.

Reference(for units 5 &6)

1. F.L. Pilar, *Elementary Quantum Chemistry*, McGraw-Hill,1968.
2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson EducationInc.,
3. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics,* 4th Edition, Oxford University Press,2005.
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7. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc.,1993.
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10. C.N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry*, PrisBooks Pvt.Ltd.,1998.

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

FCHE2C06: CO-ORDINATION CHEMISTRY

(3Credits, 54hrs)

COs	COURSE OUTCOMES
CO1	To summarize the stability of co-ordination compounds.
CO2	To categorize the different theories about Co-ordination compounds.
CO3	To explain the electronic spectra, magnetic properties characterization of Co-ordination compounds.
CO4	To discuss the different mechanisms for the reaction mechanism in metal complexes.

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 pH-metry 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 fields. Factors affecting crystal field splitting. Spectrochemical and nephelauxetic series.Racahparameters.Jahn-Teller effect.Molecular orbital theory-composition of ligand group orbitals.MO diagram of octahedral, tetrahedral and square planar complexes.π-bonding and molecular orbital theory.

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

Types of magnetic properties-Paramagnetism and diamagnetism. Curie and Curie-Weiss laws.The$\mu_{J,}$ $\mu_{L+S,}$ 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 coordination complexes.ESR spectra – application to copper complexes. NMR spectroscopy for structural studies of diamagnetic metal complexes from chemical shift and spin- spin coupling. Mossbauer spectroscopy- the Mossbauer effect, hyperfine interactions (qualitative treatment). Application to iron and tin compounds.

Unit 5: Reaction Mechanism of Metal Complexes (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 labilitybyAdamson`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.
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M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER II

FCHE2C07: REACTION MECHANISM IN ORGANIC CHEMISTRY

(3 Credits, 54 hrs)

COs	**COURSE OUTCOMES**
CO1	To compare and contrast the different mechanisms of substitution, addition, elimination reactions.
CO2	To discuss the different kinds of reaction intermediate, its formation, stability and reactions.
CO3	To summarize the different reactions of carbonyl and related compounds.
CO4	To apply different methods for explaining the outcome of a Pericyclic reaction.
CO5	To explain the photochemistry of organic compounds.

Unit I: Aliphatic Substitution Reactions (6 h)

Aliphatic nucelophilic substitution reactions – saturated and unsaturated systems – Mechanism of nucleophilic substitution – S_N2, S_N1 – ion pairs, SET, Neighbouring group participation – non classical carbocations. Substitution at allylic and vinylic carbon atoms. Effect of substrate structure, attacking nucleophile, leaving group and reaction medium on reactivity and regioselectivity.

Aliphatic Electrophilic substitutions: S_E1 S_E2 and S_Ei mechanisms with suitable examples.

Unit II: Addition and Elimination Reactions (9h)

Addition to carbon-carbon multiple bonds: Mechanistic and stereochemical aspects of reactions involving electrophiles, nucleophiles and free radicals. Electrophilic addition-Markovnikov's and anti-Markovnikov's addition, Hydroboration, Hydroxylation. Nucleophilic addition-Michael addition. Addition to cyclopropane ring.

Elimination Reaction: Mechanistic and stereochemical aspects of E1, E2 and E1cB eliminations. The effect of substrate structure, base, leaving group and reaction medium on elimination reactions. Saytzev*vs* Hofmann elimination, Bredt's rule, α- elimination, pyrolytic *syn*elimination (E*i*) – Chugaev reaction and Cope elimination. Dehydration of alcohols, Dehalogenation of vicinal dihalides and Peterson elimination.

UNIT III. Chemistry of Carbocations and Nitrenes (6 h)

Generation, structure, stability and characteristic reactions of carbocations. Classical and non-classical carbocations. C-X bond (X = C, O, N) formations through the intermediary of carbocations.

Generation, structure, stability of nitrenes. Characteristic reactions - Cycloaddition to alkenes, arenes, C-H bond insertions and rearrangement reactions.

Unit IV: Chemistry of Carbanions (9 h)

Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond (X = C,

O, N) formations through the intermediary of carbanions. Chemistry of enolates and enamines - Stork-enamine reactions. Kinetic and Thermodynamic enolates. − lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates. Named reactions under carbanion chemistry-Aldol, Claisen, Reformatsky, Perkin, Stobbe, Darzen, Knoevenagel, Dieckmann and Thorpe condensations.

Unit V: Chemistry of Free Radicals and Carbenes (9 h)

Generation of radical intermediates and its reactions. Formation of carbon-halogen bonds -

substitution in saturated compounds, substitution in allylic and benzylic compounds by NBS

and decarboxylative bromination (Hunsdiecker reaction). C−C bond formation − Addition to

alkenes, alkynes (inter and intra molecular), coupling of alkynes, McMurry coupling. C−N

bond formation – Hofmann-Loffler-Freytag reaction, Barton reaction. C-O bond formation –

Autooxidation.

Generation, structure, stability of carbenes. Characteristic reactions - Cyclopropanation - spin dependence and stereochemistry, carbene insertion to C-H bonds. Rearrangement reactions of ofcarbenes – Wolf rearrangement.

Unit VI: Molecular Rearrangements (15 h)

Unifying principles and mechanisms of rearrangements taking place at an electron deficient and electron rich substrates.

Rearrangements taking place at electron deficient carbon

(1)Pinacol-Pinacolone rearrangement (2) Semipinacol rearrangement (3) Wagner-Meerwein rearrangement (4) Tiffeneu-Demjanov rearrangement (5) Dienone phenol rearrangement (6) Wolff rearrangement.

Rearrangements at electron deficient nitrogen

(1) Hofmann (2) Curtius (3) Lossen (4) Schmidt (5) Beckmann

Rearrangements at electron deficient oxygen

(1) Baeyer Villiger (2) Dakin's reaction

Rearrangements at electron rich carbon

(1) Wittig (2) Favorskii (3) Stevens (4) Neber

Aromatic rearrangements

(1) Benzidine (2) Fries (3) Von Richter (4) Sommelet-Hauser

References:

1. R. Bruckner, *Advanced Organic Chemistry: Reaction Mechanism*, Academic Press, 2002.
2. F.A. Carey, R.A. Sundberg, *Advanced Organic Chemistry, Part B: Reactions and Synthesis*, 5/e., Springer, 2007.
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10. Jie Jack Li, *Name reactions*, 3/e, Springer.

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

FCHE2C08: MOLECULAR SPECTROSCOPY

(3 Credits, 72h)

COs	COURSE OUTCOMES
CO1	To discuss the various branches of spectroscopy like rotational spectroscopy, vibrational spectroscopy, Raman and electronic spectroscopy.
CO2	To describe and interpret the magnetic nature of certain nuclei.
CO3	To apply the concepts of vibrational, electronic, NMR and mass spectroscopy in organic molecules.

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

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

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

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

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

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

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

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

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

Electron Spin Resonance: Quantum mechanical description of electron spin in a magnetic field, Energy levels-Population- Transition probabilities using Ladder operators, g factor hyperfine interaction, Mc Connell Relation, Equivalent and non-equivalent nucleus, g anisotropy, Zero field splitting -Kramer's theorem.

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

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

UV-Visible spectroscopy: Factors affecting the position and intensity of electronic absorption bands – conjugation, solvent polarity and steric parameters. Empirical rules for calculating λ_{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 configurationof 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 classes of organic compounds hydrocarbons,alcohols, thiols, carbonyl compounds, amines, nitriles.

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

1HNMR: Chemical shift, factors influencing chemical shift, anisotropic effect. Chemical shift values of protons in common organic compounds, chemical, magnetic and stereochemical equivalence. Enantiotopic, diasteriotopic and homotopic protons. Protons onoxygen 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 orderNMR spectra.

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

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

13C NMR: General considerations, comparison with PMR, factors influencing carbon chemical shifts, carbon chemical shifts and structure-saturated aliphatics, unsaturated aliphatics, carbonyls, and aromatics. Off-resonance and noise decoupled spectra,Introduction to DEPT, INEPT, INADEQUATE.

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

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

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

References: For Units 1, 2, 3 & 4

1. G.M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw Hill, 1962.

2. C.N. Banwell& E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill, New Delhi,1994.

3. Thomas Engel, *Quantum Chemistry & Spectroscopy*, Pearson education, 2006.

4. P. Atkins & J. De Paula, *Atkins's Physical Chemistry*, 8th Edition, W.H. Freeman & Co.,2006.

5. D.A. McQuarrie and J.D. Simon, *Physical Chemistry - A Molecular Approach*, University Science Books, 1997.

6. D.N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*,UniversityPress, 2000.

7. R.S. Drago, *Physical methods for Chemists,* Second edition, Saunders College Publishing 1977 (For NMR and EPR,Mossbauer)

8. Gunther, NMR Spectroscopy: Basic Principles, Concepts and Applications inChemistry,2/e,– John Wiley

9. Ferraro, Nakamoto and Brown, Introductory Raman Spectroscopy, 2/e, Academic Press, 2005.

For Units 5, 6, 7 & 8

1. Lambert, Organic Structural Spectroscopy,2/e,Pearson

2. Silverstein, Spectrometric Identification of Organic Compounds, 6/e,John Wiley

3. Pavia, Spectroscopy, 4/e, Cengage

4. Jag Mohan, Organic Spectroscopy: Principles and Applications,2/e,Narosa

5. Fleming, Spectroscopic Methods in Organic Chemistry, 6/e, McGraw-Hill

6. P S Kalsi, Spectroscopy of organic compounds, New Age International,2007

7. William Kemp, Organic Spectroscopy, 3e, Palgrave, 2010

M.Sc. CHEMISTRY – SEMESTER I &II

FCHE2L01– INORGANIC CHEMISTRY PRACTICALS– I

(3 Credits)

COs	COURSE OUTCOMES
CO1	To apply the principles of solubility product and common-ion effect to separate and identify cations in the given mixture.
CO2	To appreciate the different types of volumetric methods for the quantitative analysis of metal ions.
CO3	To apply the basic principles of Colorimetry for the quantitative analysis of metal ions.

UNIT 1: Inorganic Cation Mixture Analysis

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

UNIT 2: Volumetric Analysis

Volumetric Determinations using:

(a) EDTA (Al, Ba, Ca, Cu, Fe, Ni, Co, hardness of water)

(b) Cerimetry (Fe2+,nitrite)

(c) Potassium Iodate (Iodide,Sn^{2+})

UNIT 3: Colorimetric Analysis

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

References

1. G.H. Jeffery, J. Basseett, J. Mendham andR.C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, 5th Edition, ELBS, 1989.

2. D.A. Skoog and D.M. West, *Analytical Chemistry, an Introduction*, 4th Edition, CBS Publishing Japan Ltd., 1986.

3. E.J. Meehan, S. Bruckenstein and I.M. Kolthoff and E.B. Sandell, *Quantitative Chemical Analysis*, 4th Edition, The Macmillan Company,1969.

4. R.A. Day (Jr.) and A.L. Underwood, *Quantitative Analysis*, 6th Edition, Prentice Hall of India, 1993.

M.Sc. CHEMISTRY – SEMESTER I &II

FCHE2L02– ORGANIC CHEMISTRY PRACTICALS– I

(3 Credits)

COs	COURSE OUTCOMES
CO1	To appreciate the different methods for the purification and separation of organic compounds.
CO2	To formulate and perform the different methods for the separation of organic binary mixtures.
CO3	To perform two stage and three stage organic preparations

Unit 1: Laboratory Techniques

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

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

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

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

References:

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

2. Shriner, FusonandCartin, *Systematic Identification of Organic Compounds*, 1964.

3. Fieser, *Experiments in Organic Chemistry*, 1957.

4. Dey, Sitaraman and Govindachari, *A Laboratory Manual of Organic Chemistry*, 3rdEdition, 1957.

5. P.R. Singh, D.C. Gupta, and K.S. Bajpal, *Experimental Organic Chemistry*, Vol. I and II, 1980.

6. Vishnoi, *Practical Organic Chemistry*.

7. Pavia, Kriz, Lampman, and Engel, *A Microscale Approach to Organic Laboratory Techniques*, 5/e, Cengage, 2013.

8. Mohrig, Hammond and Schatz, *Techniques in Organic Chemistry: Miniscale, Standard Taper Microscale and Williamson Microscale*, 3/e, W. H. Freeman and Co., 2010.

M.Sc. CHEMISTRY – SEMESTER I & II

FCHE2L03– PHYSICAL CHEMISTRY PRACTICALS – I

(3 Credits)

COs	COURSE OUTCOMES
CO1	To determine heat of the solution using thermodynamic methods.
CO2	To gain an insight into the phase diagram of eutectic, binary systems.
CO3	To apply the principles of viscosity to determine the molecular weight of polymers.
CO4	To perform refractometric analysis, different types of potentiometric and conductometrric titrations.

SECTION A

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

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

Unit 2: Phase Equilibria (minimum 3 experiments)

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

Unit 3: Viscosity (minimum 2 experiments)

1. Viscosity of mixtures - Verification of Kendall's equation (e.g., benzene- nitrobenzene, water-alcohol).
2. Determination of molecular weight of a polymer (e.g., polystyrene)

Unit 4: Distribution Law (minimum 3 experiments)

1. Determination of distribution coefficient of I2 between CCl4 and H2O.
2. Determination of equilibrium constant of KI + I2 =KI3
3. Determination of concentration of KI solution.

SECTION B

Unit 5: Refractometry (minimum 3 experiments)

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

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

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

Unit 6: Conductivity (minimum 4 experiments)

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

2. Determination of solubility product of a sparingly soluble salt (e.g., AgCl,BaSO4)

3. Conductometric titrations

(a) HCl vs NaOH

(b) (HCl + CH3COOH) vs NaOH

4. Determination of the degree of hydrolysis of aniline hydrochloride

Unit 7: Potentiometry (minimum 3 experiments)

1. Potentiometric titration: HCl vs NaOH, CH3COOH vs NaOH

2. Redox titration: KI vs KMnO4, FeSO4 vs K2Cr2O7

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

4. Determination of pH of weak acid using Potentiometry

5. Determination of pH of acids and bases using pHmeter

Reference:

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

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

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

4.F.Daniel,J.W.Williams,P.Bender,R.A.Alberty,C.D.CornwellandJ.E.Harriman, *Experimental Physical Chemistry,* McGraw Hill, 1970.

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

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

7. J. B. Yadav, *Advanced Practical Physical Chemistry*, *Goel Publications* 8. 9. , 1989.

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

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

FCHE3C09 - ELECTROCHEMISTRY, SOLID STATE CHEMISTRY ANDSTATISTICAL THERMODYNAMICS

(4 Credits, 54h)

COs	COURSE OUTCOMES
CO1	To compare the basic aspects of equilibrium electrochemistry and dynamic electrochemistry.
CO2	To explain the electronic and optical properties of solids.
CO3	To apply the principles of statistical thermodynamics to evaluate the properties of systems.

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

The nature of electrolytes, Ion activity, Ion-ion and ion-solvent interaction, The electrical potential in the vicinity of an ion, Electrical potential, and thermodynamic functions. The Debye-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 in solution.

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

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

Unit 2: Dynamic Electrochemistry (9h)

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

UNIT 3: Solid State – I (9h)

Crystal symmetry: Symmetry elements and symmetry operations, mathematical proof for the non-existence of 5-fold axis of symmetry, crystal systems, Bravaislattices 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 cell contents. Imperfections in solids - point, line and plane defects, non-stoichiometry.

UNIT 4: Solid State – II (9h)

Electronic structure of solids: free electron theory, band theory & Zone theory, Brillouin zones; Electrical properties: electrical conductivity, Hall effect, dielectric properties, piezo electricity, ferro-electricity and ionic conductivity.

Superconductivity- Meissner effect, brief discussion of Cooper theory of superconductivity. Optical properties: photo conductivity, luminescence, colour centers, lasers, refraction & birefringence. Magnetic properties: diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism& ferrimagnetism. Thermal properties - thermal conductivity & specific heat

Unit 5: Statistical Thermodynamics- I (9h)

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

Unit 6: Statistical Thermodynamics- II (9h)

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

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

Reference:

For Units 1-4

1. D. R. Crow, *Principles and Applications of Electrochemistry*, Chapman and Hall London, 1979.

2. J.O.M. Bockrisand A.K.N. Reddy, *Modern Electrochemistry, Vol. I and II*, Kluwer Academic / Plenum Publishers, 2000.

3. Carl. H. Hamann, A. Hamnett, W.Vielstich, *Electrochemistry 2nd edn.* , Wiley- VCH, 2007.

4. Philip H Reiger, *Electrochemistry 2nd edn.* , Chapman & Hall, 1994.

5. Praveen Tyagi, *Electrochemistry,* Discovery Publishing House, 2006.

6. D.A. McInnes, *The Principles of Electrochemistry*, Dover publications, 1961.

7. L.V. Azaroff, *Introduction to Solids*, McGraw Hill, NY, 1 960.

8. A.R. West, *Basic Solid State Chemistry 2nd edn. ,* John Wiley & Sons, 1999.

3. A.R. West, *Solid State Chemistry & its Applications,* John Wiley & Sons, 2003 (Reprint2007).

4. Charles Kittel, *Introduction to Solid State Physics, 7th edn*, John Wiley &Sons, 2004 (Reprint2009).

5. Mark Ladd, *Crystal Structures: Lattices & Solids in Stereo view*, Horwood, 1999.

6. Richard Tilley, *Crystals & Crystal Structures*, John Wiley & Sons, 2006.

7. C. Giacovazzo (ed.) *Fundamentals of Crystallography 2nd edn* ., OxfordUty. Press, 2002.

8. Werner Massa, *Crystal Structure Determination 2nd edn.* , Springer2004.

9. N.B. Hanna, *Solid state Chemistry,* PrenticeHall

For Units 5 & 6

1. G.S. Rush Brooke, *Statistical mechanics,* Oxford UniversityPress.

2. T.L. Hill, *Introduction to statistical thermodynamics,* Addison Wesley.

3. K. Huary, *Statistical mechanics, Thermodynamics and Kinetics,* JohnWiley.

4. O.K.Rice, *Statistical mechanics, Thermodynamics and Kinetics,* Freeman and Co.

5. F.C. Andrews, *Equilibrium statistical mechanics,* John Wiley and sons, 1963.

6. M.C. Guptha, *Statistical Thermodynamics* , Wiley eastern Ltd.,1993

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

FCHE3C10 - ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY

(4 Credits, 54h)

COs	COURSE OUTCOMES
CO1	To classify and describe the different types of organometallic compounds.
CO2	To discuss the different type of reactions by organometallic compounds.
CO3	To explain the different aspects of metal clusters.
CO4	To describe the role of various metal ions in living systems.

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. Organometallic Polymers. 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. 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.

Cisplatin and related complexes, auranofin and arthritis treatment, vanadium complexes in medicine, lithium and mental health.

Diagnostic agents- Technetium Imaging Agents and Gadolinium MRI Imaging Agents.

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.vanLeeuwen, *Homogeneous Catalysis*, Springer,2010.S.J. Lippard and J.M.Berg, *Principles of Bioinorganic Chemistry*, University ScienceBooks.

14. I. Bertini, H.B. Grey, S.J. Lippard and J.S.Valentine, *Bioinorganic Chemistry, Viva Books Pvt. Ltd.,1998.*

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

FCHE3C11 –PHOTOCHEMISTRY AND PERICYCLIC REACTIONS

(4 Credits, 54hrs)

COs	**COURSE OUTCOMES**
CO1	Apply the concepts of pericyclic reactions in predicting the mechanism of new systems
CO2	Apply the concepts of photochemistry to various chemical and physical processes.
CO3	Generate an understanding of the synthesis of natural products.
CO4	Compare the structure and functions of biomolecules

UNIT I: Pericyclic reactions (9 h)

Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3 butadiene, 1,3,5-hexatriene andallyl system. Definition, types and classification of pericyclic reactions. Theoretical models of pericyclic reactions - Orbital correlation method, Transition state aromaticity method, Frontier molecular orbital method. Electrocyclic reactions – conrotatory and disrotatory motions: 4n, 4n+2 and allyl systems. Cycloaddition –antarafacial and suprafacial additions, [2+2] additions of ketenes, substituent effects on reactivity, regioselectivity and stereochemistry of Diels-Alder reactions. Catalysis of Diels-Alder reactions by lewis acids. Scope and synthetic applications of the Diels-Alder reaction. 1,3-dipolar cycloadditions, and cheleotropic reactions. Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, *ene*reaction. Sigmatropic shifts involving carbon moieties: [3,3]- and [5,5]- sigmatropic rearrangement, Claisen, Cope and aza-Cope rearrangements.

Unit - II: Principles of Photochemistry (9hrs)

Principles of photochemistry: Electronic states and transitions, selection rules, modes of dissipation of energy (Jablonski diagram), quantum yield. Electronic energy transfer: photosensitization and quenching process.

Photochemical reactions - Dimerisation of Anthracene, H_2-Br_2 reactions and H_2-Cl_2 reactions, Photopolymerization, Principles of utilizations of solar energy –Solar cells and their working, Photochemical processes - Radiative and non-radiative transitions - Jablonski Diagram, Chemiluminiscence, Photoluminiscence, Bioluminiscence, Thermoluminiscence, Cathodoluminiscence. Fluoroscence, Theory of Fluoroscence, Stokes, Anti-Stokes and Resonance Fluorescence. Sensitised Fluoroscence, Quenching of Fluoroscence, Stern-Volmer equation (derivation).

UNIT III: Photochemical Reactions (9 hr):

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

Unit IV: 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. Structure elucidation of atropine and quinine. Terpenoids — Isolation and classification of terpenoids. Structure of steroids. Classification of steroids. Conversion of Cholesterol to testosterone. Chemistry and stereochemical features involved in the total synthesis of Longifolene (Corey's synthesis), Reserpine and Cephalosporine C.

Unit V: Chemistry of Heterocyclic Compounds (9 h)

Basic principles of heterocyclic synthesis involving cyclisation reactions and cycloadditions.

(i) Three-membered and four-membered heterocycles: Synthesis of aziridines, oxiranes, thiranes, azetidine, oxetanes and thietanes. *(i) Five-membered heterocycles containing one hetero atom:* Synthesis and reactions of pyrroles, furans, thiophens, reduced pyrroles, reduced furans and reduced thiophens. *(ii) Five-membered heterocycles containing two heteroatoms:* Synthesis of pyrazole, imidazole, oxazole, isoxazole and thiazole. *(iii) Five-membered heterocycles containing three heteroatoms***:** Synthesis of 1,2,3-triazole and 1,2,4-tetrazole. (iv) Five-memberedheterocycles containing four hetero atoms: Synthesis of Tetrazoles.

Unit VI: Biomolecules (9 h)

Amino acids, peptides and proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures, α- helix, β-sheets, super secondary structure. Tertiary structure of protein: folding and domain structure. Quaternary structure. Nucleic acids: Structure and function of physiologically important nucleotides (c-AMP,ADP, ATP) and nucleic acids (DNA and RNA), replication, genetic code, protein biosynthesis, mutation.

References:

1. S. Sankararaman, *Pericyclic Reactions-A Textbook: Reactions, Applications and Theory*,Wiley VCH, 2005.
2. Fleming, *Molecular Orbitals and Organic Chemical Reactions*, Wiley, 2009.
3. J. Sing and J. Sing, *Photochemistry and Pericyclic Reactions*, 3/e, New Age
4. International, 2012.
5. G. M. Loudon, *Organic Chemistry*, 4/e, Oxford University Press, 2008
6. K. K. Rohtagi-Mukherji, *Fundamentals of Photochemistry*, Wiley- Eastern.
7. J. Coxon and B. Halton, *Organic Photochemistry*, Cambridge University Press.
8. A. Cox and T. Camp, *Introductory Photochemistry*, McGraw-Hill.
9. R. P. Kundall and A. Gilbert, *Photochemistry*, Thomson Nelson.
10. A. Gilbert and J. Baggott, *Essentials of Molecular Photochemistry*, Blackwell Scientific, Publication.
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13. R. R. Gupta, M. Kumar and V. Gupta, *Heterocyclic Chemistry Vol. 1-3*, Springer Velag.
14. J. A. Joules and K. Mills, *Heterocyclic Chemistry*, 4/e, Oxford University Press, 2004.
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17. N. R. Krishnaswamy, *Chemistry of Natural Products: A Laboratory Hand Book*, 2/e, Universities Press.
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21. G. L. Patrick, *An Introduction to Medicinal Chemistry*, 3/e, Oxford University Press, 2005.

22. David L. Nelson and Michael M. Cox, *Lehninger*, *Principles of Biochemistry*,6/e WH-Freeman.

23. Jeremy M Berg, John L Tymoczko and LubertStryer, *Biochemistry*, 5/e, WHFreeman.

24. U. Satyanarayana and U. Chakrapani, *Essentials of Biochemistry*, 2/e, 2012.

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

FCHE3E01- SYNTHETIC ORGANIC CHEMISTRY (Elective)

(3 Credits, 54 h)

COs	COURSE OUTCOMES
CO1	Apply main group and transition metallic reagents to the synthesis of complex organic compounds
CO2	Able to justify the selection of one reagent over another in terms of efficacy in relation to a particular synthetic problem
CO3	Predict the mechanisms of standard chemical reactions, with a focus on functional group conversions
CO4	Design synthesis of organic molecules using retro-synthetic analysis

Unit I: Reagents for Oxidation (9 h)

Oxidation of organic compounds with reagents based on peroxides, peracids, ozone, Chromium, Manganese, Osmium, Ruthenium, Alumnium, Silver, Dimethyl sulfoxide Selenium dioxide and DDQ. Oxidations of (a) alcohols to carbonyls using Chromium, Manganese and Aluminium metal based reagents. Oppenauer oxidation, Swern oxidation, Etard oxidation and Dess Martin oxidation. (b) Alkenes to epoxides (peroxides/per acids based) (c) Alkenes to diols – $KMnO_4$ and OsO_4, Woodward and Prevost hydroxylation. (d) Alkenes to carbonyls with bond cleavage – ozonolysis, Lemieux reagent, $Pb(OAc)_4$ (e) Alkenes to alcohols/carbonyls without bond cleavage hydroboration- oxidation, selenium/chromium based allylic oxidation. (f) Oxidation of ketones – □,□-unsaturated ketones, □-hydroxy ketones, oxidation to ester/lactones–Baeyer-Villiger oxidation. (g) Oxidation of allylic and benzylic C-H bonds: DDQ and SeO_2.

Unit II: Reagents for Reduction (9 h)

(a) Catalytic hydrogenation (heterogeneous and homogeneous), the catalyst, selectivity of reaction of functional groups, stereochemistry and mechanism. (b) Reduction by dissolving metals: reduction of carbonyl compounds, reduction with metal in liquid ammonia (Birch reduction), reductive cleavage. (c) Reduction by hydride transfer reagents: Aluminium alkoxides - MPV reduction, $LiAlH_4$, $NaBH_4$, and its derivatives like diisobutylaluminium hydride (DIBAL-H), sodium cyanoborohydride etc. Lithium aluminium hydride-aluminium chloride reagents. Reduction with borane and its derivatives. (d) Other methods of reduction:

Enzyme catalyzed, Wollff- Kishner reduction, Clemmenson reduction, desulphurization of thioacetals, reductions withdiimide and shapiro reaction. Reductions with trialkylsilanes.

Unit III: Synthetic Reagents (9 h)

Organometallic Reagents: Preparation and application of the following in organic synthesis - Grignard, Organo lithium and Organo copper reagents, Gilman's reagent (lithium dimethyl cuprate). Reagents based boron (organo boranes), tin - Tri-n-butyl tin hydride, and chromium –Benzene Tricarbonyl Chromium. Organo silicon reagents - trimethylsilyl iodide or chloride, synthesis of alkenes – Peterson reaction.

Use of following reagents in organic synthesis and functional group transformation: diazomethane, polyphosphoric acid, DCC (dicyclohexylcarbondioxide), Tebbe's reagent.

Unit IV. Coupling Reactions (9 h)

Coupling Reactions: Palladium catalysts for C−C, C−N and C−O bond formation, Palladium

catalyzed amine arylation (mechanism and synthetic applications). Sonogashira cross coupling reaction (mechanism and synthetic applications in Cyclic peptides), Stillecarbonylative cross coupling reaction (mechanism and synthetic applications). Mechanism and synthetic applications of Negishi, Hiyama, Kumada, Heck and Suzuki-Miyaura coupling

reactions. Buchwald-Hartwig coupling reaction.

Unit V: Chemistry of Carbonyl Compounds (9 h)

Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides, and amides. Substitution at α-carbon, aldol and related reactions. Mannich, Prins and Tischenko reaction. Conjugate additions, Michael additions and Robinson annulation. Reaction with phosphorous and sulfurylides – Wittig reaction and Horner Wadsworth Emmons modification.

Unit VI: Synthetic Strategies (9 h)

Retrosynthetic analysis: target, synthon, synthetic equivalent, disconnection approach, functional group inter-conversion (FGI), functional group addition, functional group elimination. Protection and deprotection of the following functional groups: hydroxyl, carbonyl, amino and carboxyl with applications. Importance of order of events in organic synthesis, one group and two group C−X disconnections, chemo selectivity, reversal of polarity, cyclisation reactions.

One group C−C disconnections−alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

Two group C−C disconnections – Diels-Alder reaction, 1,3-difunctionalised compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Mannich bases as intermediates in organic synthesis. Michael addition and Robinson annulations. Synthetic routes based on retrosynthetic analysis of Longifolene (Corey's synthesis).

References:

1. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4/e, Cambridge University Press.
2. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, Part B, 5/e, Springer, 2007.
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10. P. Wyatt and S. Warren, *Organic Synthesis: Strategy and Control,* Wiley.
11. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press, 2011.
12. J. J. Li, *Name Reactions*, 4/e, Springer, 2009.
13. T. W. Greene and P. G. M. Wuts: *Protecting Groups in Organic Synthesis*, 2nd ed., Wiley
14. E. J. Corey and Xue-Min Cheng, *The Logic of Chemical Synthesis,* Wiley Interscience.
15. K. C. Nicolaou and E. J. Sorensen, *Classics in Total Synthesis*, Weinhem: VCH, 1996.

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

FCHE3E02 - COMPUTATIONAL CHEMISTRY (Elective)

(4 credits, 54 h)

COs	COURSE OUTCOMES
CO1	Compare the different methods used in computational chemistry
CO2	Insight into the structure of Gaussian file and how it is applied to find molecular parameters

Unit 1: Introduction to Computational Chemistry (9 h)

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

Classification of computational methods.

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

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

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

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

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

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

UNIT 5: Density Functional Methods (9 h)

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

UNIT 6: Basis Set Approximation (9 h)

Hydrogen-like, Slater-type & Gaussian type basis functions, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization & diffuse basis sets, even tempered &well-tempered basis sets, contracted basis sets, Pople-style basis sets and their nomenclature, correlation consistent basis sets, basis set truncation error, effect of choice of method/ basis set (model chemistries) on cpu time.

References:

1. C. J. Cramer, *Essentials of computational Chemistry: Theories and models*, John Wiley & Sons 2002.
2. Frank Jensen, *Introduction to Computational Chemistry*, John Wiley & Sons LTD1999.
3. J. Foresman &Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.
4. David Young, *Computational Chemistry- A Practical Guide for Applying Techniques to Real- World Problems"*, Wiley -Interscience, 2001.
5. Errol G. Lewars, *Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics,* 2 nd edn, Springer2011.
6. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc., 2009.
7. P.W. Atkins & R.S. Friedman, *Molecular quantum mechanics*, 4th Edition, Oxford University Press, 2005.
8. W. Koch, M.C. Holthausen, *"A Chemist's Guide to Density Functional Theory"*, Wiley-VCH Verlag 2000.

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

FCHE3E03 - INDUSTRIAL CATALYSIS
(Elective)

(4 Credits, 54h)

COs	COURSE OUTCOMES
CO1	To summarize different types of adsorption, its kinetics and theories.
CO2	To describe the preparation, deactivation of catalyst surfaces.
CO3	To analyse the role of phase transfer catalyst and Bio-catalyst in catalysis.
CO4	To apply the principles of catalysis for conducting different organic reactions in macro scale.

Unit 1: Introduction to Adsorption process (9h)

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

Unit 2: Kinetics and Catalysis (9h)

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

References:

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

2. J.M. Thomas & W.J. Thomas, *"Introduction to principles of heterogeneous catalysis",* Academic Press, New York, 1967.

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

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

Unit 3: Catalyst – Activation and Deactivation (9h)

Surface area and porosity measurement. Measurement of acidity of surfaces. Support materials. Preparation and structure of supports. Surface properties. Preparation of catalysts. Introduction of precursor compound. Pre-activation treatment. Activation process. General methods of synthesis of zeolites. Mechanism of nuclear formation and crystal growth. Structures of some selected zeolites. Zeolites A, X and Y. Pentasils. ZSM-5. ZSM-11. Shape selective catalysis by zeolites. Deactivation of catalysts. Classification of catalyst deactivation processes. Poisoning of catalysts. Coke formation on catalysts. Metal deposition on catalysts. Sintering of catalysts. Regeneration of deactivated catalysts. Feasibility of regeneration. Description of coke deposit and kinetics of regeneration.

References:

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

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

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

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

UNIT 4: Phase Transfer Catalysis (9h)

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

UNIT 5: Biocatalysis (9h)

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

References:

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

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

UNIT 6: Industrial Catalysis (9h)

Oil based chemistry. Catalytic reforming. Catalytic cracking. Paraffin cracking. Naphthenic cracking. Aromatic hydrocarbon cracking. Isomerization. Hydrotreatment. Hydrodesulphurization. Hydrocracking. Steam cracking. Hydrocarbons from synthesis gas. Fisher-Tropsch process. Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources. Hydroformylation of olefins. Carbonylation of organic substrates. Conversion of methanol to acetic acid. Synthesis of vinyl acetate and acetic anhydride. Palladium catalyzed oxidation of ethylene. Acrylonitrile synthesis. Zeigler-Natta catalysts for olefin polymerization. Propene polymerization with silica supported metallocene/MAO catalysts.

References:

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

2. R.J. Farrauto and C.H. Bartholomew, *"Fundamentals of Industrial Catalytic Processes",* Blackie Academic and Professional – Chapman and Hall, 1997.

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

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

FCHE4C12- INSTRUMENTAL METHODS OF ANALYSIS

(4 Credits, 72 h)

COs	**COURSE OUTCOMES**
CO1	To summarize different methods for the treatment of statistical data.
CO2	To compare the volumetric and gravimetric methods of quantitative analysis.
CO3	To describe the different types of electro-analytical techniques, optical, thermal and radiochemical methods used in chemical analysis.
CO4	To classify and analyse different chromatographic methods in qualitative and quantitative analysis.

Unit 1: **Errors in Chemical Analysis (9h)**

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

Unit 2: **Conventional Analytical Procedures (9h)**

Gravimetry: **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-l-naphthol, dithiocarbamates. Acid-Base and precipitation titrations: theory of neutralisation titrations, indicators for acid/base titrations, titration curves of strong acid, strong base, weak acid, weak base and polyprotic acids. Buffer solutions. Titrations in nonaqueous media. Different solvents and their selection for a titration. Indicators for nonaqueous titrations.

Redox titrations: Permanganometry, dichcrometry, iodometry, cerimetry. Variation of potential during a redox titration, formal potential during a redox titration, Redox indicators. Precipitation titrations, adsorption indicators.

Complexometric titrations: Types of EDTA titrations (direct, back, replacement, alkalimetric and exchange reactions), masking and demasking agents, selective demasking, metal ion indicators - murexide, eriochrome black T, Patton and Reeder's indicators, bromopyrogallol red, xylenol orange, variamine blue.

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

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

Unit 4 Electro Analytical Methods II (9h)

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

Unit 5 Optical Methods - I (9 h)

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

Atomic absorption spectrometry: sample atomization techniques, instrumentation, interferences, background correction, and analytical applications.

Unit 6 Optical Methods - II (9 h)

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

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

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

Unit 8: Chromatography (9 h)

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

basic instrumental set up-carriers, columns, detectors and comparative study of TCD, FID, ECD and NPD. Qualitative and quantitative studies using GC, Preparation of GC columns, selection of stationary phases of GLC, Gas adsorption chromatography, applications, CHN analysis by GC.

References:

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

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

a. 9th Edn ., Cengage Learning., 2014.

3. J.G. Dick, *Analytical Chemistry*, R.E. Krieger Pub.,1978.50

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

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

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

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

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

10. H.A. Laitinen, W.E. Harris, *Chemical Analysis*, McGraw Hill, 1975.

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

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

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

a. Edition, Wiley-VCH, 2006.

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

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

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

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

20. 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, 2005 6841-6851.

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

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

FCHE4E04 - PETROCHEMICALS AND COSMETICS (Elective)

(4Credits, 72h)

COs	COURSE OUTCOMES
CO1	Study the various processes involved in the refining of petroleum
CO2	Apply the concept of petroleum refining in designing novel technologies with better efficiency
CO3	Compare the cosmetics and prepare a list of ingredients in the commercially available samples

Unit 1: Introduction to Petrochemistry (9h)

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

Unit 2: Hydrocarbons from Petroleum (9h)

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

Unit 3: Industrial Organic Synthesis (9h)

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

Unit 4: Composition of Petroleum Crude (9h)

Composition of petroleum crude. Composition of the petroleum products. Isomeric compounds. Classification of petroleum crude. A survey of the world crude. Sulphur compounds in petroleum. Physical Properties and Test Methods. 1. Viscosity: Other methods for finding out viscosity. Viscosity of an oil blend. Use of the figure for finding out viscosity. Viscosities of hydrocarbons. 2. Density, 3. Surface and interfacial tensions. 4. Refractive Index. 5. Flash and fire points. 6. Cloud and pour points. 7. Aniline point. 8. Diesel index. 9.

Cetane number. 10. Octane number and knock characteristics. 11. Distillation curves. (a) ASTM (American Society for Testing Materials) distillation curve. (b). Hempel or semi fractionating distillation curve.

Unit 5: Distillation of Crude Petroleum (9h)

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

Unit 6: Petroleum Products (9h)

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

Unit 7: Purification of Petroleum Products (9h)

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

Unit 8: Perfumes and Cosmetics (9h)

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

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

Cosmetics: Economics and Advertising.

References:

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

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

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

4. Uttam Ray Chaudhuri, *"Fundamentals of Petroleum and Petrochemical Engineering",* Boca Raton London New York.

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

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

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

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

FCHE4E05 – SUPRAMOLECUALR, MEDICINAL & GREEN CHEMISTRY (Elective)

(4 Credits, 72 hrs)

COs	COURSE OUTCOMES
CO1	Study emerging branches in chemistry like supramolecular chemistry, medicinal chemistry, heterocyclic chemistry and its applications
CO2	Apply the principles of green chemistry to devise alternate pathway for the conventional organic reactions
CO3	To compare the recent advancement in reagents and synthetic methods
CO4	To get an overview about research process and to gain the ability to apply various research methods and techniques

Unit I: Supramolecular chemistry (12 h)

Definition and development of supramolecular chemistry, nature of supramolecular interactions - hydrogen bonding, dipole-dipole, charge transfer, van der Waals and π-π stacking interactions.

Concepts in supramolecular chemistry: Supramolecular hosts and molecular recognition – factors and forces involved in molecular recognition, classification of molecular receptors (crown ethers, cryptands, spherands, cyclodextrins and calixarenes). Bi.omimetics and catalysis Supramolecular devices – molecular switches, wires and motors. Mechanically-interlocked molecular architectures (catenanes and rotaxanes).

Molecular self-assembly – Factors responsible for self-assembly; Liquid crystals, gels and dendrimers as self-assembled systems. Self-assembled monolayer (SAM) as an example for controlled self-assembly.

Applications of supramolecular chemistry – Molecular sensors, Materials technology, Catalysis, Medicine, Data storage and processing.

Unit II: Green Chemistry (6 h)

Green chemistry – relevance and goals, twelve principles of green chemistry – Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples. Comparison of traditional process versus green process in the synthesis of ibuprofen.

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

Use of the following in synthesis with suitable examples: (a) Green catalysts: Phase transfer catalysts [Tetra-n-butyl ammonium chloride, benzyltrimethyl ammonium chloride (TMBA), Aliquat 336], crown ethers and biocatalysts. (b) Green solvents: water, ionic liquids and supercritical fluids. (c) Polymer supported reagents and synthesis – Properties of polymer support, Advantages of polymer supported reagents. Applications – Synthesis of peptides (Merrifield solid-phase peptide synthesis), synthesis of oligonucleotide and oligosaccharides.

(d) Microwave assisted synthesis. (e) Ultrasound assisted reactions.

Unit IV: New reactions in organic synthesis (9 h)

(a) C=C Formation Reactions: Bamford-Stevens reaction, Shapiro reaction, Julia olefination and Peterson olefination.

(b) Ring Formation Reactions: Pauson-Khand reaction, Bergman cyclisation and Nazerov cyclisation, Tiffeneau–Demjanov rearrangement.

(c) Multicomponent Reactions: Biginelli synthesis; multicomponent reactions using alkyl isocyanides−Passerini and Ugi-4-component synthesis.

(d) Olefin metathesis using Grubb's catalyst.

(e) Other important synthetic reactions: Mukaiyama esterification, Mitsunobu reaction and Baylis Hillman reaction.

Unit V: New techniques and Concepts in organic synthesis (9 h)

Combinatorial synthesis: Basic ideas and concepts of combinatorial chemistry.

Click Chemistry: Criteria for click reaction, Sharplessazides cycloadditions.

Domino/Cascade reactions: Introduction and applications in organic synthesis.
Baldwin Rules: Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations

Unit VI: Medicinal Chemistry and Drug design (9 h)

Theories of drug activity: Occupancy theory, rate theory and induced fit theory, General Principles of dosage form design and drug administration, Pharmacokinetics, pharmacodynamics, metabolites and antimetabolites, Prodrugs and parmacophores, agonists and antagonists, Drug design, factors governing drug design, rational approach to drug design, the design of agonists, the design of antagonists, Concept of drug receptor, Elementary treatment of drugs receptor interaction, Quantitative structure activity relationship (QSAR), General methods of drug synthesis, Synthetic strategies, stereochemistry, combinatorial library synthesis.

Unit VII: Six-membered Heterocyclic & Fused Ring Heterocyclic Compounds (9 h)

Six-membered Heterocyclic Compounds: (i) Six-membered heterocycles containing one heteroatom: Synthesis and reactions of pyridine. synthesis of pyrones and pyrylium salts. (ii) Six-membered heterocycles containing two hetero atoms: Synthesis of pyridazines, pyrimidines (uracil, thymine and cytosine), pyrazines. Synthesis of purines- adenine and guanine. (iii) Six-membered heterocycles containing three hetero atoms: Synthesis of 1,3,5-triazines, 1,2,3-triazines and 1,2,4-triazines.

Fused ring hetero cyclic compounds: Structure and synthesis of benzofuran, indole, isoindole, benzothiophene, quinoline, isoquinoline, benzoxazole, benzthiazole and benzimidazole. Structure and synthesis of azepines, oxepines, thiepins, diazepines and benzodiazepines. Structure and synthesis of uric and caffeine

Unit VIII: Research methodology in Chemistry (9 h)

Science and scientific method.The choice and statement of a research problem. Searching the

literature. Literature databases − Google scholar, SciFinder, Web of science, PubMed, INFLIBNET etc. Formulation of hypothesis. Research plans. Design of experiment. Design of apparatus. The execution of experiments. Analysis of the experimental data. Interpretation and generalization of the findings. Patenting and reporting the results of research. Scientific writing – research reports, journal articles, books and thesis. Type of journal publications−articles, communications, reviews. Organization of reports – general format, the title, authors, abstract, text (introduction, method, results, discussion, conclusions), acknowledgement, references. Abbreviations, foot notes, Tables, Figures, Proof reading. Important scientific and chemistry journals. Impact factor.

References:

1. K. Ariga and T. Kunitake, *Supramolecular Chemistry — Fundamentals and Applications*, Springer, 2006.
2. Jonathan W. Steed and Jerry L. Atwood, *Supramolecular Chemistry*, 2/e, Wiley, 2009.
3. J. M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, 1995.
4. F. Vogtle, Supramolecular Chemistry: An Introduction, Wiley, 1993.
5. V. K. Ahluwalia, *Green Chemistry: A Textbook*, Narosa Publishing House, 2013.
6. *Green Chemistry – Designing Chemistry for the Environment* – edited by Paul T. Anastas& Tracy C. Williamson. Second Edition, (1998).
7. V. K. Ahluwalia and R. Aggarwal, *Organic synthesis – Special Techniques*, 2/e, Narosa.
8. W. Carruthers, *Some modern methods of organic synthesis*, Cambridge University Press.
9. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, Part B, 5/e, Springer, 2007.
10. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, 3/e, CRC Press, 1998.
11. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 2/e, Oxford University Press, 2012.
12. N. K. Terret: *Combinatorial Chemistry*, Oxford University Press, 1998.
13. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press, 2011.
14. J. J. Li, *Name Reactions*, 4/e, Springer, 2009.
15. Gringuaz Alex, *Introduction to medicinal chemistry*, New York: Wiley-VCH, 1996.
16. S. N. Pandeya and J. R. Dimmock, *An introduction to drug design*. New Age International.
17. *Richard B. Silverman and Mark W. Holladay, The organic chemistry of drug design and drug action*, 3/e, Elsevier.
18. Lednicer Daniel, *Strategies for organic drug synthesis and design*, 2/e, John Wiley, 2008.
19. Patrick Graham, *Instant notes in medicinal chemistry*, Taylor & Francis.
20. G. R. Chatwal, *Medicinal Chemistry*, Himalaya, 2002.
21. J. Richard Smith and Michael L, *Analysis of Drug Impurities*, John Wiley & Sons, 2007.
22. Thomas L. Gilchrist, *Heterocyclic chemistry*, 3/ e, Pearson Education, 2007.
23. R. R. Gupta, M. Kumar and V. Gupta, *Heterocyclic Chemistry Vol. 1-3,* SpringerVelag.
24. J. A. Joules and K. Mills, *Heterocyclic Chemistry*, 4/e, Oxford University Press, 2004.

25. R. Kartritzky and C. W. Rees, *Comprehensive Heterocyclic Chemistry, Vol-1-7*, Pergamon press.
26. R. L. Dominoswki, *Research Methods*, Prentice Hall, 1981.
27. J.W. Best, J.V. Kahn, *Research in Education*, 10thEdn., Pearson/Allyn& Bacon, 2006.
28. H. F. Ebel, C. Bliefert, W.E. Russey, *The Art of Scientific Writing*, Wiley-VCH, 2004.

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

FCHE4E06 - NATURAL PRODUCTS & POLYMER CHEMISTRY (Elective)

(4 Credits, 72 h)

COs	COURSE OUTCOMES
CO1	To apply the principles of organic synthesis for the structural elucidation of terpenoids, steroids, alkaloids, anthocyanins.
CO2	To summarize the basic aspects about dyes, pigments and Supramolecules.
CO3	To appreciate different types of polymerisation techniques.
CO4	To discuss the stereochemistry and various characterization techniques for polymers.
CO5	To describe the basic aspects of speciality polymers.

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

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

UNIT 2: Terpenoids and Steroids (9 h)

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

UNIT 3: Alkaloids and Anthocyanins (9 h)

Alkaloids. Classification of alkaloids, structural elucidation based on degradative reactions (quinine and atropine). Biosynthesis of quinine and papaverine.

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

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

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

References:

1. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press, 2011.
2. F. A. Carey and R. J. Sundberg*: Advanced Organic Chemistry (part B),* 3rd ed., Plenum Press.
3. T.W. G. Solomons: *Fundamentals of Organic Chemistry*, 5th ed., John Wiley
4. H. O. House: *Modern Synthetic Reactions*, W. A. Benjamin
5. W. Carruthers: *Some Modern Methods of Organic Synthesis*, 4/e, Cambridge University 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, Oxford University Press
8. N. R. Krishnaswamy: *Chemistry of Natural Products*; A Unified Approach, Universities Press
9. R. J. Simmonds: *Chemistry of Biomolecules: An Introduction*, RSC
10. R. O. C. Norman: *Principles of Organic Synthesis*, 3nd ed., CRC Press, 1998.
11. J. M. Lehn, *Supramolecular Chemistry*

UNIT 5: **Polymerization Processes (9 h)**

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

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

Polymer Stereochemistry. Organizational features of polymer chains. Configuration and conformation, Tacticity, Repeating units with more than one asymmetric center. Chiral polymers – main chain and side chain. Stereoregular polymers. Manipulation of polymerization processes.

Zeigler-Natta and Kaminsky routes. Coordination polymerization. Metallocene and Metal oxide catalysts. Polymer Characterization. Molecular weights. Concept of average molecular weights, Molecular weight distribution. Methods for determining molecular weights. Static and dynamic methods, Light scattering and GPC. Crystalline and amorphous states. Glassy and Rubbery States. Glass transition and crystalline melting. Spherullites and Lammellac. Degree of Crystallinity, X-ray diffraction.

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

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

Copolymers. EVA polymers. Flourine containing polymers. Polyacetals. Reaction polymers.

Polyamides, polyesters. Epoxides, polyurethanes, polycarbonates, phenolics, PEEK, Silicone polymers.

UNIT 8: **Speciality Polymers (9 h)**

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

References:

1. F.W. Billmayer. *Textbook of Polymer* Science. 3rd Edn, Wiley. N.Y. 1991.
2. G. Odiyan, *Principles of Polymerisation*, 4/e, Wiley, 2004.
3. V.R. Gowriker and Others, *Polymer Science*, Wiley Eastern Ltd.
4. J.M.G Cowie. *Polymers: Physics and Chemistry of Modern Materials*. Blackie. London, 1992.
5. R.J.Young, *Principles of Polymer Science*, 3rd Edn. , Chapman and Hall. N.Y. 1991.
6. P.J. Flory. *A Text Book of Polymer Science.* Cornell University Press. Ithacka, 1953.
7. F. Ullrich, *Industrial Polymers*, Kluwer, N.Y. 1993.
8. H.G.Elias, *Macromolecules*, Vol. I & II, Academic, N.Y. 1991.

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

FCHE4E07 - MATERIAL SCIENCE
(Elective)

(4 credits, 72hrs)

COs	COURSE OUTCOMES
CO1	To categorize different methods for the preparation of Nano materials.
CO2	To illustrate different techniques used for the characterisation of Nano Materials.
CO3	Describe the preparation, deactivation of catalyst surfaces.
CO4	Analyse the role of phase transfer catalyst and Bio-catalyst in catalysis.
CO5	Apply the principles of catalysis for conducting different organic reactions in macro scale

Unit 1: Nanomaterials (9hrs)

History of nanomaterials- Classification. Size- dependence of properties. Electronic structuretheory of metals and semiconductors. Quantum size effects. Synthesis of nanostructures: bottom-up-approach, top- down approach, self-assembly, lithography, molecular synthesis, template assisted synthesis. Nanocomposites.

Unit 2: Characterisation and Applications of Nanomaterials (9hrs)

Methods of characterization: Electron microscopies- SEM, TEM. Scaning probe 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 unit 1& 2):

1. G. Cao, Nanostructures & Nanomaterials: Synthesis, Properties & Applications,Imperial College Press, 2003
2. C.N.R. Rao, Nanoworld: An Introduction to Nanoscience & Technology,Navakarnataka Publications Pvt Ltd, 2014
3. T. Pradeep, *The essentials of Nanotechnology*, Tata McGraw Hill, New Delhi,2007.

4. C.P. Poole (Jr.) and F.J. Owens, *Introduction to Nanotechnology*,WileyIndia,2007.
5. G.A. Ozin and A.C. Arsenault, *Nanochemistry*, RSC Publishing, 2008.
6. K.J. Klabunde(Ed.), *Nanoscale Materials in Chemistry*, John Wiley&Sons,2001.
7. G. L. Hornyak, H.F. Tibbals, J. Dutta, J.J. Moore, Introduction to Nanoscience and Nanotechnology, CRC Press, 2008

Unit 3: Industrial Heterogeneous Catalysis (9hrs)

Introduction to Phase transfer catalysis, bio catalysis, nano catalysis and polymer supported catalysis. Application of heterogeneous catalysts in water gas shift reaction, ammonia synthesis, catalytic cracking, zeolites based heterogeneous catalysis. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

References

1. Dipak Kumar Chakrabarty, *Adsorption and Catalysis by Solids*, New Age. 2007.
2. C.H. Bartholomew and R.J. Farrauto, *Fundamentals of Industrial Catalysis Process,* 2nd Edn.Wiley& Sons Inc. 2006.
3. Woodruff, D. P. and Delchar T. A., *Modern Techniques of Surface Science*, Cambridge Solid State Science Series, 1994.
4. Kurt K. Kolasinski, *Surface Science: Foundations of Catalysis and Nanoscience*, 3rd Edn.,Wiley U. K., 2012.

Unit 4: **Polymerization Processes I (9 hrs)**

Polymerization processes. Free radical addition polymerization. Kinetics and mechanism.Chaintransfer.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.

Unit 5: Polymerization Processes II (9 hrs)

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.

Unit 6: 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.Poly anilines, poly pyrrols, poly thiophines, poly (vinylenephenylene).Photoresponsive and photorefractive polymers.Polymers in optical lithography. Polymer photo resists. Electrical properties of Polymers, Polymers with NLO properties, second and third harmonic generation, wave guide devises.

References for Unit 4, 5&6

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

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

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

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

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

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

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

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

Unit 7: Composite Materials (9hrs)

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

Unit 8: Fracture Mechanics (9hrs)

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

References:

1. A.G. Guy, *Essentials of Material Science*, McGrawHill.
2. M.J. Starfield and Shrager, *Introductory Material Science*, McGrawHill.
3. S.K. HajraChoudhary, *Material Science and Engineering*, Indian Book Dist. Co., Calcutta.
4. F.R. Jones, *Handbook of Polymer Fibre Composites*, Longman Scientific andTech.
5. K.K. Chowla, *Composite Materials*, Springer-Verlag, NY, 1987.

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

FCHE4E08 – ORGANOMETALLIC CHEMISTRY (Elective)

(4 credits, 72h)

COs	COURSE OUTCOMES
CO1	To classify and describe the different types of organometallic compounds.
CO2	To discuss the different type of reactions by organometallic compounds.
CO3	To explain the different aspects of metal clusters.

UNIT I (9h)

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

UNIT II (9h)

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

UNIT III (9h)

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

UNIT IV (9h)

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

UNIT V (9h)

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

UNIT VI (9h)

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

UNIT VII (9h)

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

UNIT VIII (9h)

Organometallic Polymers. Polymers with organometallic moieties as pendant groups. Polymers with organometallic moieties in the main chain. Condensation polymers based on ferrocene and on rigid rod polyynes, poly (ferrocenylsilane)s, applications of oly(ferrocenylsilane)s and related polymers. Applications of rigid-rod polyynes, polygermanes and polystannanes. Polymers prepared by ring opening polymerization. Organometallic dendrimers.

References:

1. B. D. Gupta, A .J. Elias, Basic Organometallic Chemistry - Concepts, Synthesis and Applications, Second edition, University Press, 2013.
2. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, Fourth edn. 2005, Wiley Interscience.
3. J. E. Huheey, Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, Pearson education, 1993.
4. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry. 5th edition, John and Wiley, 1999.
5. R.S. Drago. Physical Methods in Inorganic Chemistry, 2nd edition, affiliated east west press, 1993.
6. P. Powell, Principles of Organomettalic Chemistry, 2nd edition, Chapman and Hall,

London, 1998.

7. S. F. A. Kettle, Concise co-ordination chemistry, Nelson, 1969.
8. S. F. A. Kettle, Physical Inorganic Chemistry-A Co-ordination chemistry Approach, Spectrum academy publishers, 1996.
9. Purcell and Kotz, Inorganic Chemistry. 10. D. J. Shriver, P. W. Atkins, Inorganic Chemistry, 5th edition, Oxford university press, 2010.

M.Sc. CHEMISTRY – SEMESTER III & IV

FCHE4L04 – INORGANIC CHEMISTRY PRACTICALS– II

(3 Credits)

COs	COURSE OUTCOMES
CO1	To apply the gravimetric and colorimetric methods to separate and quantitatively analyse the inorganic ions present in it.
CO2	To perform ion-exchange methods for the separation and estimation of binary mixtures.
CO3	To generate inorganic complexes.

Unit 1: Estimation of ions in mixture

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

Unit 2: Colorimetric Estimations

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

Unit 3: Ion Exchange Methods

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

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

References:

1. *Vogel's Text Book of Qualitative InorganicAnalysis*.

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

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

4. W.G.Palmer, *Experimental InorganicChemistry.*

5. G. Brauer, *Hand book of Preparative InorganicChemistry*.

M.Sc. CHEMISTRY – SEMESTER III & IV

FCHE4L05– ORGANIC CHEMISTRY PRACTICALS– II

(3 Credits)

COs	COURSE OUTCOMES
CO1	To apply the different methods of organic analysis for the quantitative analysis of amino acids, vitamins and antibiotics.
CO2	To perform extraction and purification of natural products.
CO3	To apply the chromatographic technique for the analysis of natural products.

Unit 1: Quantitative Organic Analysis

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

References:

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

2. Beebet, *Pharmacuetical Analysis*.

Unit 2: Extractions

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

Unit 3: Chromatograhy

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

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

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

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

Plant growth stimulants: Indole acetic acid.

References:

1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, 5/e, Pearson, 1989.
2. Beebet, *PharmacueticalAnalysis*
3. E. Hoftmann, *Chromatography*, non Nostrand Reinhold Company, New York, 1975.
4. J. Sherma and G. Zwig, *TLC and LC analysis of pesticides of international importance*, Vol. VI & VII, AcademicPress.
5. H. Wagner, S. Bladt, E.M. Zgainsti – Tram, Th. A. Scott., *Plant Drug Analysis*, Springer- Verlag, Tokyo,1984.
6. Vishnoi, *Practical Organic Chemistry*.

M.Sc. CHEMISTRY – SEMESTER III & IV

FCHE4L06– PHYSICAL CHEMISTRY PRACTICALS– II

(3 Credits)

COs	COURSE OUTCOMES
CO1	To apply the concepts of chemical kinetics and Polarimetry to determine the rates of chemical reactions.
CO2	To apply the concepts of adsorption to verify isotherms.
CO3	To design phase diagram for different type of systems.
CO4	To apply the principles of spectrophotometry for the quantitative analysis of metals.
CO5	To apply the different methods of computational chemistry to calculate the molecular properties.

SECTION A

Unit 1: Chemical Kinetics (4 experiments)

1. Determination of specific reaction rate of acid hydrolysis of an ester (methyl acetate or ethyl acetate) and concentration of the given acids.
2. Determination of Arrhenius parameters of acid hydrolysis of an ester.
3. Determination of specific reaction rate of saponification of ethyl acetate.
4. Iodination of acetone in acid medium – Determination of order of reaction with respect of iodine and acetone.

Unit 2: Adsorption (3 experiments)

1. Verification of Langmuir adsorption isotherm – charcoal-acetic acid system. Determination of the concentration of a given acetic acid solution using the isotherm
2. Verification of Langmuir adsorption isothem – charcoal-oxalic acid system. Determination of the concentration of a given acetic acid solution using the isothem.
3. Determination of surface area of adsorbent.

Unit 3: Phase Equilibria (2 experiments)

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

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

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

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

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

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

1. Determination of cyroscopic constant of a liquid (water, benzene)
2. Determination of molecular mass of a solute (urea, glucose, cane sugar, mannitol) by studying the depression in freezing point of a liquid solvent (water, benzene)
3. Determination of Van't Hoff factor and percentage of dissociation of NaCl.
4. Study of the reaction 2Kl + Hgl2 →.K2Hgl4 and determination of the concentration of the given Kl solution.

Unit 5: Polarimetry (3 experiments)

1. Determination of specific and molar optical rotations of glucose, fructose and sucrose.
2. Determination of specific rate of inversion of cane sugar in presence of HCl.
3. Determination of concentration of HCl

Unit 6: Spectrophotometry (3 experiments)

1. Determination of equilibrium constants of acid –base indicators.
2. Simultaneous of determination Mn and Cr in a solution of KMnO4 and K2Cr2O7
3. Investigation of complex formation between Fe (III) and thiocyanate.

References:

1. A. Finlay and J.A. Kitchener, *Practical Physical Chemistry,* Longman.
2. F. Daniels and J.H. Mathews, *Experimental Physical Chemistry,* Longman.
3. A.H. James, *Practical Physical Chemistry*, J.A. Churchil Ltd., 1961.
4. H.H. Willard, L.L. Merit and J.A. Dean, *Instrumental Methods of Analysis,* 4th Education, Affiliated East-West Press Pvt. Ltd., 1965.
5. D.P. Shoemaker and C.W. Garland, *Experimental Physical Chemistry,* McGrawHill.
6. J.B. Yadav, *Advanced Practical Physical Chemistry, Goel Publications,* 1989

SECTION B

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

Unit 7: Computational Chemistry Calculations

1. Single point energy calculations of simple molecules like H2O and NH3 at the HF/3-21G level of theory.
2. The effect of basis set on the single point energy of H2O and NH3 using the Hartree-Fock

method (3-21G, 6-31G, 6-31+G, 6-31+G* basis sets can be used).

3. Geometry optimization of molecules like H2O, NH3, HCHO & C2H4 at the HF/6-31G level of theory.
4. Computation of dipole and quadrupole moments of HCHO & C2H4 at the HF/6-31G level of theory.
5. Effect of basis set on the computation of H-O-H bond angle in H_2O using the Hartree-Fock method (3-21G, 6-31G, 6-31+G, 6-31+G* basis sets can be used).
6. Computation of the energy of HOMO and LUMO of formaldehyde and ethylene at the HF/6-31G level of theory.
7. Effect of substituent (F & Cl) on the geometric parameters (like C-C bond length) of ethylene at the HF/6-31G level of theory.
8. Comparison of stability of cis-planar and trans-planar conformers of H2O2 at the HF/6-31G level of theory.
9. Comparison of stability of cis- and trans- isomers of difluoroethylene at the HF/6-31G* level of theory.
10. Computation of the frequencies of normal modes of vibration of molecules like H2O, NH3 and CO2 at the HF/6-31+G* level of theory.
11. Determination of hydrogen bond strength of H2O dimer and H2O trimer at the HF/6-31+G* level of theory.
12. Determination of hydrogen bond strength of HF dimer and HF trimer at the HF/6-31+G* level of theory.

Reference:

1. J. Foresman &Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.
2. David Young, *Computational Chemistry- A Practical Guide for Applying Techniques to Real- World Problems"*, Wiley -Interscience, 2001.
3. http://classic.chem.msu.su/gran/gamess/index.html