UNIVERSITY OF CALICUT
G & A - IV - K SECTION

No. 194023/GA-IV-K-ASST-2/2024/Admn (I) Calicut University.P.O

Dated: 10.06.2026

From

The Registrar

To

The Principal
Sacred Heart College (Autonomous)
Chalakudy

Sir/Madam,

Sub:- Syllabus of M.Sc Chemistry programme w.e.f 2024 Admission onwards-Approved-reg

Ref:- 1. Communication received from the Principal of Sacred Heart College (Autonomous), Chalakudy

2. Remarks of the Chairperson, BoS in Chemistry(PG).

3. Orders of the Vice-Chancellor, dated 09.06.2026

With reference to the above, this is to inform that the Board of Studies in Chemistry (PG) vide reference cited (2) above, has approved the syllabus of **M.Sc Chemistry programme w.e.f 2024 admission onwards**, submitted by Sacred Heart College (Autonomous), Chalakudy.

The Vice-Chancellor has approved the above resolution of the Board of Studies. Please find the approved syllabus attached for your reference.

Yours faithfully
Arsad M
Deputy Registrar
(For The Registrar)

Copy to

PA to CE / DR, BSc Branch

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

M. Sc. DEGREE PROGRAMME
IN
CHEMISTRY

w.e.f 2024 Admissions onwards

SCHEME AND SYLLABUS

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

M.Sc. CHEMISTRY (CBCSS PATTERN)

Regulations and Syllabus with effect from 2024 admission

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

Theory Courses

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

Practical Courses

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

Project and Viva Voce

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

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

Grading and Evaluation

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

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

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

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

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

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

Letter Grade	Grade Range	Range of Percentage (%)	Merit / Indicator
O	4.25 – 5.00	85.00 – 100.00	Outstanding
A+	3.75 – 4.24	75.00 – 84.99	Excellent
A	3.25 – 3.74	65.00 – 74.99	Very Good
B+	2.75 – 3.24	55.00 – 64.99	Good
B	2.50 – 2.74	50.00 – 54.99	Above Average
C	2.25 – 2.49	45.00 – 49.99	Average
P	2.00 -2.24	40.00 – 44.99	Pass
F	< 2.00	Below 40	Fail
I	0	-	Incomplete
Ab	0	-	Absent

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

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

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

(4) Weightage of Internal and External valuation:

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

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

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

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

Theory: 5 weightage

a) Internal Examinations- weightage = 2 (2 internal exams, both should be considered)

b) Assignments and Exercises- weightage=1

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

Practical: 10 weightage

a) Attendance - weightage=2
b) Lab. skill/quality of their results- weightage=2
c) Model practical test-weightage= 2
d) Record – weightage =2
e) Viva Voce- weightage=2

Project: 10 weightage

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

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

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

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

(6) External evaluation:

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

Pattern of question Papers for theory courses is as follows

Division	*Type*	*No.of Questions*	*Weightage*	*Total Weightage*
Section A	Short Answer	8 out of 10	1	8
Section B	Short Essay	6 out of 8	2	12
Section C	Essay	2 out of 4	5	10
	Total weightage in a question paper		**30**	

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

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

Component	Weightage
Physical & Theoretical Chemistry – theory courses	5

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

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

a) 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 project is 4.

(7) Directions for question paper setters:

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

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

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

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

(Further details regarding the grading and evaluation are as per the Sacred Heart College (Autonomous) College PG regulations 2024)

Chairman

(Sacred Heart (Autonomous) College|)

Audit courses:

Ability Enhancement Courses(AEC):

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

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

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

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

After conducting the AEC, the evaluation/examination should be done either common for all students in a batch or individually depending upon the AEC conducted. The evaluation/ examination must be conducted jointly by the teacher in charge of the AEC and the head of the department. The result of the AEC, duly signed and sealed by both teacher in charge and head of the department, should be uploaded to the Office of the Controller of the examination 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 Office of the Controller of the examination. Evaluation/examination on AEC must contain the following components: MCQ type written examination, Report on AEC, Presentation of AEC, Viva voce on AEC. Distribution of 30 weightage may be done by the teacher in charge in concurrence with the Head of the department.

Professional Competency Course (PCC):

This course particularly aims to improve the skill level of students, especially for using specific as well as nonspecific software useful in their respective field of study, both related to the core and elective subject area. Also, it is a platform for the student community to undertake socially committed projects and thereby developing a method of leaning process by through the involvement with society.

PCC is a 4 credit course and should be conducted during the second semester of the programme. The credit of the PC course will not be considered while calculating the SGPA/CGPA.

But the student has to obtain minimum pass requirements in this course, which is compulsory for an overall pass in the programme

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

a) Development of skills on using softwares like Gaussian, Gamess etc which is useful in molecular modeling, drug designing, etc.
b) Development of skills on using softwares like Chemdraw, Chem window, 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, 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.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.

But the student has to obtain minimum pass requirements in this course, which is compulsory for an overall pass in the programme

MSc CHEMISTRY

PROGRAMME SPECIFIC OUTCOMES

	Programme Specific Outcomes
PSO 1	Apply the fundamental principles of analytical, inorganic, organic, and physical chemistry to explain chemical phenomena and solve scientific problems.
PSO 2	Conduct research projects by formulating research objectives, performing experiments, analyzing data, and interpreting results.
PSO3	Demonstrate safe handling of chemicals and evaluate environmental, energy, health, and medicinal issues using chemical knowledge.
PSO 4	Communicate and present conceptual and applied chemical knowledge effectively to academic, professional, and societal audiences.
PSO 5	Apply chemical knowledge to design experiments and integrate fundamental concepts with applications in research, industry, academia, and medicine.
PSO 6	Employ critical thinking and scientific methods to design, perform, record, analyze, and interpret chemical experiments.
PSO 7	Implement the principles of green chemistry and promote environmentally sustainable practices in chemical processes and daily life.

TABLE 1
Courses offered for M.Sc. Chemistry Programme under CBCSS Pattern in Sacred Heart College(Autonomous), Chalakudy

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

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

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY
(4Credits, 72 hours)

COURSE OUTCOME

COURSE: QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY
COURSE CODE: CHE1C01
Credits: 4
Total hours: 72
4hrs/week

	Course outcome	POs/ PSOs	COGNITIVE LEVEL	KNOWLEDGE CATEGORY
1	Explain the postulates of quantum mechanics and their significance in describing microscopic systems.	PSO I	U	P
2	Analyze the quantum mechanical treatment of a one-dimensional box, three-dimensional box, and simple harmonic oscillator.	PSO I	U	C
3	Explain the quantum mechanical models of a particle on a ring and a particle on a sphere.	PSO I	E	F
4	Determine the eigenfunctions and eigenvalues of hydrogen-like atoms and interpret their physical significance.	PSO II	E	P
5	Analyze and apply approximate methods used in quantum mechanics to solve chemical problems.	PSO I	An	P

6	Explain the concepts of many-electron systems and the antisymmetry principle.	PSO I	E	C
7	Compare and contrast the fundamental principles of Molecular Orbital (MO) and Valence Bond (VB) theories.	PSO I	An	F
8	Apply Hückel theory to analyze conjugated π-electron systems.	PSO I	E	P
9	Explain and predict hybridization and molecular geometry in chemical systems.	PSO II	U	P
10	Perform and evaluate computational calculations using the Gaussian software package.	PSO II	E	P

Total hours of instruction 72

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A))**

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, orthonormality of wave functions; Operator postulate, operator algebra, linear and nonlinear operators, Non-commuting operators and the Heisenberg's Uncertainty principle, Laplacian operator, Hermitian operators and their properties, eigen functions and eigen values of an operator; Eigen value postulate, eigen value equation, Expectation value postulate; Postulate of time- dependent Schrödinger equation of motion, conservative systems and time-independent Schrödinger equation.Stationary states.

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

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

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

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

Co-ordinate systems: - Cartesian, and spherical polar coordinates and their relationships. Planar rigid rotor (or particle on a ring), the Phi-equation, solution of the 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, Ladder operator method for angular momentum, space quantization.

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 spin functions.

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 (9hrs)

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

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

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,Oxford University Press,2005.
4. M.W. Hanna, *Quantum Mechanics in Chemistry*, 2nd Edition, W.A. Benjamin Inc., 1969.
5. Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983 (first Indian edition,Viva books,2003).
6. Thomas Engel, Quantum Chemistry & Spectroscopy, Pearson Education,2006.
7. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc.,1993.
8. Horia Metiu, *Physical Chemistry – Quantum Mechanics*, Taylor & Francis,2006.
9. A.K. Chandra, *Introduction to Quantum Chemistry* , 4th Edition, Tata McGraw-Hill, 1994.

10. L. Pauling and E.B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1935 (A good source book for manyderivations).
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*, 2nd edn., Springer2011.

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

COURSE OUTCOME

COURSE : INORGANIC CHEMISTRY I(4 Credits, 72hrs)
COURSE CODE : CHE1CO2
Credits: 4

	Course outcome	POs/ PSOs	CL	KC
1	Analyze the properties, applications, and significance of nanochemistry and nanomaterials.	PSO III	An	F
2	Explain the principles and methods used for the synthesis of nanostructures.	PSO II	U	C
3	Compare and interpret the major acid-base theories and their applications in chemical systems.	PSO III	U	C
4	Apply Wade's rules to predict and evaluate the structures of electron-deficient boron compounds.	PSO I	E	C
5	Explain and analyze the structure, bonding, and synthesis of P–N, P–S, and S–N compounds.	PSO II	U	C
6	Construct and interpret Ellingham, Latimer, Frost, and Pourbaix diagrams for chemical systems.	PSO I	An	P
7	Compare and evaluate the theories proposed to explain nuclear structure.	PSO I	U	C
8	Explain and analyze the interaction of radiation with matter and its chemical consequences.	PSO II	U	F

Total hours of instruction 72

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A))**

Unit 1: Concepts of Acids and Bases (12hrs)

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 –surface acidity.

Unit 2: Chemistry of Main Group Elements-I (12hrs)

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

Allotropes of C, S, P. As, Sb, Bi, O and Se. Electron deficient compounds-Boron hydrides-preparation, reactions, structure and bonding. Styx numbers-closo, nido, arachno polyhedral structures. Boron cluster compounds-Wade's rule. Polyhedral borane anion-carboranes, metallaboranes and metallacarboranes. Borazines andborides.

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Unit 3: Chemistry of Main Group Elements-II(12hrs)

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

Unit 4: Chemistry of Transition and Inner Transition Elements (12hrs)

Heteropoly and isopoly anions of W, Mo, V.

Standard reduction potentials and their diagrammatic representations Ellingham diagram. Latimer and Frost diagrams. Pourbaix diagram.

Differences between 4f and 5f orbitals. Magnetic and spectroscopic properties. Uranyl compounds. Trans-actinide elements. Super heavy elements –production and chemistry.

Unit 5: Nuclear and Radiation Chemistry (12hrs)

Structure of nucleus: shell, liquid drop, Fermi gas, collective and optical models.

Nuclear reaction: Bethe`s notation of nuclear process- Types-reaction cross section- photonuclear and thermonuclear reactions.

Nuclear fission: Theory of fission- neutron capture cross section and critical size.

Nuclear fusion. Neutron activation analysis

Radiation chemistry: Interaction of radiation with matter. Detection and measurement of radiation- GM and scintillation counters – radiolysis of water- radiation hazards- radiation dosimetry.

Unit 6: Chemistry of Nanomaterials (12hrs)

History of nanomaterials - Classification. Size- dependence of properties.

Synthesis of nanostructures: bottom-up-approach, top- down approach, self- assembly, lithography, molecular synthesis, template assisted synthesis.

Methods of characterization: Electron microscopies-SEM,TEM. Scaning prob microscopies- STM, AFM. X-ray photoelectron spectroscopy(XPS), Dynamic light scattering(DLS), X-ray diffraction(XRD).

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

Introduction to graphenes and fullerenes.

Reference (for units 1 to 5)

1. N.N. Greenwood and A.Earnshaw, *Chemistry of Elements, 2/e, Elsevier* Butterworth-Heinemann,2005.
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. H.J.Arnikar, *Essentials of Nuclear chemistry*, New Age International,2005.
9. Friedlander and J.W.Kennedy, *Introduction to Radiochemistry*, John Wiley and Sons, 1981.
10. S.Glastone, *Source Book on Atomic Energy, 3*rdedn., Affiliated East-West Press Pvt.Ltd., 1967.

Reference (for unit 6):

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

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS

COURSE OUTCOME

COURSE: STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS (4 Credits,72hrs)
COURSE CODE : CHE1CO3
Credits: 4
Total hours: 72

	Course outcome	POs/ PSOs	CL	KC
1	Explain the nature of hydrogen bonding and analyze its effects on the physical and chemical properties of organic compounds.	PSO II	U	C
2	Construct molecular orbitals of simple molecules using the Hückel method and interpret the results.	PSO I	An	C
3	Differentiate aromatic, antiaromatic, and homoaromatic systems based on molecular orbital theory.	PSO I	U	C
4	Explain the fundamental concepts and principles involved in organic reaction mechanisms.	PSO II	U	C
5	Analyze the factors influencing the conformational stability of organic molecules.	PSO I	An	F
6	Evaluate the effect of molecular conformation on the rate and course of reactions in various organic systems.	PSO II	An	C
7	Analyze and distinguish optical and geometrical isomerism in organic compounds.	PSO II	E	C
8	Explain and evaluate the concepts of chiral pool synthesis, chiral auxiliaries, and chiral reagents in stereoselective synthesis.	PSO II	U	P

Total hours of instruction 72

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A))**

Unit 1: Structure and Bonding in Organic Molecules (12 hrs)

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

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

Hückel MO method. MO's of simple molecules, ethylene, allyl radical and 1,3-butadiene. Hückel rule and modern theory of aromaticity, criteria for aromaticity and antiaromaticity, MO description of aromaticity and antiaromaticity. Homoaromaticity. Aromaticity of annulenes and heteroannulenes, fused ring systems, fulvenes, fulvalenes, azulenes, pentalenes andheptalenes. Preparation of aromatic and antiaromatic compounds by different methods, stability of benzylic cations and radicals. Effect of delocalized electrons onpKa.

Unit 2: Structure and Reactivity (12 hrs)

Transition state theory, Potential energy vs reaction co-ordinate curve, substituent effects (inductive, mesomeric, inductomeric, electomeric and field effects) on reactivity. Qualitative study of substitution effects in S_N1-S_N2 reactions. Neighbouring group participation, participation of carboxylate ion, halogen, hydroxyl group, acetoxy group, phenyl group and pi -bond. Classical and nonclassical carbocations

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

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

Unit 3: Conformational Analysis – I (12 hrs)

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

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

Unit 4: Conformational Analysis – II (12 hrs)

Effect of conformation on the course and rate of reactions in (a) debromination of dl and meso 2,3-dibromobutane or stilbene dibromide using KI. (b) semipinacolic deamination of erythro and threo 1,2-diphenyl-1-(p-chlorophenyl)-2-amino ethanol. (c) dehydro halogination of stilbene dihalide (dl and meso) and erythreo threo- bromo-1,2-diphenyl propane.

Effect of conformation on the course andrate of reactions in cyclohexane systems illustrated by: (a) S_N2 and S_N1 reactions for (i) an axial substituent, and (ii) an equatorial substituent inflexible and rigid systems. (b) E1, E2 eliminations illustrated by the following compounds. (i) 4-t-Butylcyclohexyl tosylate (cis and trans) (ii) 2-Phenylcyclohexanol (cis and trans) (iii) Menthyl and neomenthyl chlorides and benzene hexachlorides. (c) Pyrolytic elimination of esters (cis elimination) (d) Esterification of axial as well as equatorial hydroxyl and hydrolysis of their esters in rigid and flexible systems. (Compare the rate of esterification of methanol, isomenthol, neomenthol and neoisomenthol). (f) Esterification of axial as well asequatorial carboxyl groups and hydrolysis of their esters. (g) Hydrolysis of axial and equatorialtosylates. (h) Oxidation of axial and equatorial hydroxyl group to ketones by chromic acid.

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

Unit 5: Stereochemistry (12 hrs)

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

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

Optical isomerism in biphenyls, allenes and nitrogen and sulphur compounds, conditions for optical activity, R and S notations. Optical activity in cis-trans conformational isomers of 1,2-, 1,3- and 1,4-dimethylcyclohexanes.

Restricted rotation in biphenyls – Molecular overcrowding.

Chirality due to folding of helicalstructures.

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

Unit 6: Asymmetric Synthesis (12 hrs)

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

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

1. Substrate controlled asymmetric synthesis: Nucleophillic addition to chiral carbonyl compounds. 1,2-asymmetric induction, Cram's rule and Felkin-Anhmodel.
2. Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, azaenolates, imines and hydrazones, chiral sulfoxides. 1,4-Asymmetric induction and Prelog's rule. Use of chiral auxiliary in Diels-Alder and Copereactions.
3. Chiral reagent controlled asymmetric synthesis: Asymmetric reduction usingBINAL – H. Asymmetric hydroboration using IPC_2BH and $IPCBH_2$. Reduction with CBH reagent. Stereochemistry of Sharpless asymmetric epoxidation anddihydroxylation
4. Asymmetric aldol reaction: Diastereoselective aldol reaction and its explanation by Zimmermann-*Traxler* model. Auxillary controlled aldol reaction. Double diastereoselection-matched and mismatched aldol reactions

References:

1. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A,* Springer, 5/e, 2007.
2. M. B. Smith, J. March, *March's Advanced Organic Chemistry*, John Wiley & Sons, 6/e, 2007.
3. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3/e Addison-Wesley,1998.
4. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 2/e, Oxford UniversityPress,2012.
5. E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books,2005.
6. M. S. Singh, *Advanced Organic Chemistry: Reactions and Mechanisms*, Pearson,2013.
7. P. Sykes, *A Guide book to Mechanism in Organic Chemistry*, 6/e, Pearson,2006.
8. C. K. Ingold, Structure and Mechanism in Organic chemistry, 2/e, CBS Publishers, 1994.
9. E. L. Eliel, S. H. Wilen and L. N. Mander, *Stereochemistry of Carbon Compounds*, John Wiley,1997.
10. G. L. D. Krupadanam, *Fundamentals of Asymmetric Synthesis*, Universities Press, 2013.
11. Okuyama and Maskill, Organic Chemistry: A Mechanistic Approach, Oxford University Press,2013
12. S. Warren and P. Wyatt, *Organic Synthesis: The Disconnection Approach,* 2/e, John Wiley & Sons,2008.

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

COURSE: THERMODYNAMICS, KINETICS AND CATALYSIS (4 Credits, 72hrs)
COURSE CODE : CHE1CO4
Credits: 4

	Course outcome	POs/ PSOs	CL	KC
1	Apply the third law of thermodynamics to determine absolute and residual entropies of chemical systems.	PSO I	An	F
2	Analyze the thermodynamic behavior of solutions, ideal and real gases, and gaseous mixtures.	PSO II	U	C
3	Interpret and evaluate excess functions such as excess Gibbs free energy, excess entropy, excess enthalpy, and excess volume in non-ideal systems.	PSO I	U	C
4	Evaluate the validity of Onsager theory and apply it to explain diffusion phenomena.	PSO I	E	F
5	Analyze the kinetics of chain reactions, fast reactions, and reactions in solution.	PSO II	An	C
6	Explain molecular reaction dynamics using molecular beam techniques.	PSO II	U	P
7	Apply Langmuir adsorption theory and the BET equation to analyze adsorption phenomena and characterize surface topology.	PSO II	U	C
8	Compare and evaluate homogeneous and heterogeneous catalysis based on their mechanisms and applications.	PSO I	E	F

Total hours of instruction 72

(Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A))

Unit 1: Thermodynamics (12hrs)

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, Residualentropy.

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 andtheir 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 (12 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 (12 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 (12 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 (12 hrs)

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

Unit 6: Catalysis (12 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 $2CO + O_2 \longrightarrow 2CO_2$. 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.

6. K.J.Laidler, J.H.Meiser and B. C. Sanctuary, *Physical Chemistry*, Houghton Mifflin Company, New York,2003.

7. A.W. Adamson, *Physical Chemistry of surfaces,* 4th edition, Interscience, New

York,1982.

8. G. K. Vemulapalli, *Physical Chemistry*, Printice Hall ofIndia.
9. M.K. Adam, *The Physics and Chemistry of surfaces* , DoverPublications
10. S. Glasstone, *Thermodynamics for chemists,* East-West1973.
11. Rajaram and Kuriokose, *Thermodynamics*, East-West1986
12. Pigoggine, *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.* 2nd 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,* 2nd 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*, 3rd Edn., Wiley U. K.,2012

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

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

COURSE OUTCOME

COURSE: GROUP THEORY and CHEMICAL BONDING
COURSE CODE:CHE2CO5
Credits:3
Total hours: 54

	Course outcome	POs/ PSOs	CL	KC
1	Apply similarity transformation to solve symmetry-related problems in chemistry.	PSO I	An	P
2	Analyze molecular symmetry and classify molecules into appropriate point groups.	PSO II	Ap	C
3	Compare and contrast the fundamental principles of Molecular Orbital (MO) and Valence Bond (VB) theories.	PSO I	An	F
4	Apply Hückel theory to analyze conjugated π-electron systems.	PSO I	E	P
5	Explain and predict hybridization and molecular geometry in chemical systems.	PSO II	U	P
6	Construct symmetry-adapted linear combinations (SALCs) using the projection operator method.	PSO II	Ap	P
7	Classify atomic orbitals into appropriate symmetry species based on molecular symmetry.	PSO I	E	F
8	Determine and evaluate the IR and Raman active vibrational modes of molecules using symmetry principles.	PSO II	Ap	P
9	Explain and apply the Great Orthogonality Theorem in symmetry and group theoretical calculations.	PSO I	U	P
10	Construct and interpret character tables for molecular point groups.	PSO II	Ap	F

Total hours of instruction 54

(Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A) Apply (Ap))

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 of symmetry operations of a molecule, point groups and their systematic identification, GMT of point groups;

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

UNIT 2: Representations of Point Groups & Corresponding Theorems (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 – wave functions (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 Ramanspectra.
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 and H_2O as examples, classification of atomic orbitals involved into symmetry species, group orbitals, symmetry adapted linear combinations (SALC), projection operator, construction of SALC using projection operator, use of projection operator in constructing SALCs for the π MOs in cyclopropenyl ($C_3H_3^+$)cation.

Unit 5: Chemical bonding in diatomic molecule (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 homo nuclear diatomic molecules – Li_2, Be_2, C_2, N_2, O_2& F_2 and hetero nuclear diatomic molecules – LiH, CO, NO & HF, bond order, correlation diagrams, non-crossing rule; Spectroscopic term symbols for diatomic molecules; Comparison of MO and VB theories.

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

Hybridization – quantum mechanical treatment of sp, sp^2& sp^3 hybridisation; Semi empirical MO treatment of planar conjugated molecules – Hückel Molecular Orbital (HMO) theory of ethylene, butadiene & allylic anion, charge distributions and bond

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

Reference (for Units 1 to 4)

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.
5. P.H. Walton, *Beginning Group Theory for Chemistry*, Oxford University Press Inc., New York,1998.
6. Mark Ladd, *Symmetry & Group Theory in Chemistry*, Horwood1998.
7. A. Salahuddin Kunju & G. Krishnan, *Group Theory & its Applications in Chemistry*, PHI Learning Pvt. Ltd.2010.
8. Arthur M Lesk, *Introduction to Symmetry & Group theory for Chemists*, Kluwer AcademicPublishers,2004.
9. K.Veera Reddy, *Symmetry & Spectroscopy of Molecules 2nd Edn.*, New Age International 2009.
10. A.W. Joshi, *Elements of Group Theory for Physicists*, New Age International Publishers, 1997.

Reference(for units 5 &6)

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.
4. M.W. Hanna, *Quantum Mechanics in Chemistry*, 2nd Edition, W.A. Benjamin Inc., 1969.

5. Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983 (first Indian edition, Viva books,2003).

6. Thomas Engel, *Quantum Chemistry & Spectroscopy*, Pearson Education,2006.

7. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc.,1993.

8. A.K. Chandra, *Introduction to Quantum Chemistry*, 4th Edition, Tata McGraw-Hill, 1994.

9. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International,2006.

10. C.N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry*, Prism Books Pvt.Ltd.,1998.

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

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

COURSE OUTCOME

COURSE: COORDINATION CHEMISTRY
COURSE CODE : CHE2CO6
Credits: 3
Total hours: 54

	Course outcome	POs/ PSOs	CL	KC
1	Analyze the factors affecting the stability of coordination compounds.	PSO I	U	C
2	Compare and interpret the bonding in coordination complexes using VBT, CFT, and MOT.	PSO I	An	C
3	Construct molecular orbital diagrams for coordination complexes and interpret their bonding characteristics.	PSO I	Ap	F
4	Apply Orgel and Tanabe–Sugano diagrams to explain the electronic spectra and magnetic properties of coordination compounds.	PSO I	Ap	P
5	Determine and interpret the magnetic properties of coordination complexes.	PSO I	U	C
6	Characterize coordination complexes using various spectroscopic techniques and interpret the resulting data.	PSO III	Ap	P
7	Evaluate reaction mechanisms exhibited by metal complexes based on kinetic and mechanistic evidence.	PSO II	E	F
8	Compare and analyze outer-sphere and inner-sphere redox reactions in coordination complexes.	PSO I	U	P

Total hours of instruction 54

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A),Apply (Ap))**

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 templateeffects.

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. Racah parameters. Jahn-Teller effect. Molecular orbital theory-composition of ligand group orbitals. MO diagram of octahedral, tetrahedral and square planar complexes. π-bonding and molecular orbital theory.

Unit 3: Electronic Spectra and Magnetic Properties of Complexes (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 D_q, B and β parameters. Tanabe-Sugano diagrams. Charge transfer spectra.

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

Unit 4: Characterization of Coordination Complexes (9hrs)

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

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

References:

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

2 J.E.Huheey, E.A.Keiter, R.L.Keiter and O.K.Medhi, *Inorganic Chemistry, principles of structure* and *reactivity*, Pearson Education, 2006.

3. G.L.Miessler, D.A.Tarr, *Inorganic Chemistry*,Pearson,2010.

4. D.F.Shriver, P.W.Atkins, *Inorganic Chemistry*,Oxford University Press,2002

5. William W Porterfield, *Inorganic Chemistry-A unified approach,* Academic Press, 2005.

6 .Keith F Purcell, John C Kotz, *Inorganic Chemistry*, Cengage Learning, 2010.

7. James E House, *Inorganic Chemistry,* Academic Press,2008.

8. B.Douglas, D.McDaniel, J.Alexander, *Concepts and Models of Inorganic Chemistry,*Wiley Student Edition,2006.

9. A.W.Adamson and P.D.Fleischauer, *Concepts of Inorganic Photochemistry,Wiley.*

10. F.A.Cotton and G.Wilkinson, *Advanced Inorganic Chemistry*,Wiley.

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

12. R.L.Dutta and A.Shyamal, *Elements of Magnetochemistry,* S.Chand and Co.1982.

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

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

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

CHE2C07 - REACTION MECHANISM IN ORGANIC CHEMISTRY

(3 Credits, 54hrs)

COURSE OUTCOME

COURSE: REACTION MECHANISM IN ORGANIC CHEMISTRY
COURSE CODE:CHE2CO7
Credits: 3
Total hours:54

	Course outcome	POs / PS Os	CL	KC
1	Explain and differentiate aliphatic and aromatic nucleophilic and electrophilic substitution reactions with their mechanisms.	PSO II	U	C
2	Analyze the mechanisms of addition and elimination reactions involving electrophiles and nucleophiles.	PSO II	U	C
3	Compare and evaluate the stability, geometry, and reactivity of reaction intermediates.	PSO I	E	F
4	Analyze nucleophilic reactions of carbonyl compounds and predict their reaction outcomes.	PSO II	An	F
5	Explain and evaluate the mechanisms of ester hydrolysis based on experimental evidence.	PSO II	R	C
6	Apply the principles of pericyclic reactions to explain reaction pathways and stereochemical outcomes.	PSO I	U	P
7	Explain and evaluate the principles and applications of photochemical reactions in organic chemistry.	PSO I	An	F
8	Classify and compare natural products based on their structure, properties, and biological significance.	PSO I	U	C

Total hours of instruction 54

(Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A))

Unit 1: Aliphatic and Aromatic Substitutions (9 hrs)

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

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

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

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

(i) Addition and Elimination Reactions (6hrs)

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

Mechanistic and stereo chemical aspects of E1, E1cB and E2 eliminations. The effect of substrate structure, base, leaving group and reaction medium on elimination reactions. Saytzev *vs* Hofmann elimination, α-elimination, pyrolytic *syn* elimination (E*i*) and conjugate eliminations. Competition between substitution and elimination reactions, basicity *vs* nucleophilicity. Extrusion reactions-extrusion of N_2, CO andCO_2.

(ii) Reactive Intermediates (3hrs)

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

Unit 3: Chemistry of Carbonyl Compounds (9hrs)

(i) Reactions of Carbon-hetero multiple Bonds (7hrs)

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

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

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

Unit 4: Pericyclic Reactions (9 hrs)

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

Unit 5: Photochemistry of Organic Compounds (9 hrs)

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

Unit 6: Chemistry of Natural Products (9 h)

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

References:

1. M. B. Smith and J. March, *March's Advanced Organic Chemistry*, 6/e, John Wiley & Sons,2007.
2. F. A. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, *Part A & B*, 5/e, Springer,2007.
3. E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books,2005.
4. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3/e Addison-Wesley,1998.
5. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, 3/e, CRC Press, 1998.
6. Peter Sykes, *A Guide book to Mechanism in Organic Chemistry*, 6/e, Pearson,2006.
7. S. Sankararaman, *Pericyclic Reactions-A Textbook: Reactions*, *Applications and Theory*, Wiley VCH,2005.
8. I. Fleming, *Molecular Orbitals and Organic Chemical Reactions*, Wiley,2009.
9. J. Sing and J. Sing, *Photochemistry and Pericyclic Reactions*, 3/e, New Age International,2012.
10. G. M. Loudon, *Organic Chemistry,* 4/e, Oxford University Press, 2008
11. M. B. Smith, *Organic Chemistry: An Acid Base Approach*, CRC Press,2010.
12. T. Okuyama and H. Maskill, *Organic Chemistry A Mechanistic Approach*, Oxford University Press,2014.
13. I. Fleming, *Selected Organic Synthesis*, John Wiley and Sons,1982.

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

15. E. Corey and I.M. Chang, *Logic of Chemical Synthesis*, John Wiley, New York,1989.

16. I. L. Finar, *Organic Chemistry Vol 2: Stereochemistry and the Chemistry of Natural Products*, 5/e, Pearson,2006.

17. N. R.Krishnaswamy, *Chemistry of Natural Products: A Laboratory Hand Book,* 2/e, Universities Press

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

COURSE OUTCOME

COURSE: ELECTRO CHEMISTRY,SOLID STATE CHEMISTRY AND STATISTICAL THERMODYNAMICS
COURSE CODE: CHE2C08
Credits: 3
Total hours: 54
3hrs/week

	Course outcome	POs/PSOs	CL	KC
1	Explain and apply the Debye–Hückel equation in its limiting and extended forms to ionic solutions.	PSO I	U	C
2	Analyze and compare the efficiency of electrochemical cells and heat engines.	PSO I	An	C
3	Compare and evaluate the theories proposed to explain hydrogen overvoltage.	PSO I	An	F
4	Explain the principles of polarography and the operation of the Dropping Mercury Electrode (DME).	PSO I	U	F
5	Apply Bragg's law to determine crystal structures and evaluate its applications in structural analysis.	PSO I	U	C
6	Compare and analyze the electrical, thermal, magnetic, and optical properties of solids.	PSO I	An	C
7	Evaluate partition functions and relate them to thermodynamic properties of chemical systems.	PSO I	E	F
8	Compare and analyze Maxwell–Boltzmann (M–B), Bose–Einstein (B–E), and Fermi–Dirac (F–D) statistics and their applications.	PSO I	U	C

Total hours of instruction 54

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A)**

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

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

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

Unit 2: Dynamic Electrochemistry (9hrs)

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

UNIT 3: Solid State – I (9hrs)

Crystal symmetry: Symmetry elements and symmetry operations, mathematical proof for the non-existence of 5-fold axis of symmetry, crystal systems, Bravais lattices and crystal classes, Crystallographic point groups - Schönflies & Hermann–Mauguin notations, Stereographic projections of the 27 axial point groups, translational symmetry elements & symmetry operations - screw axes and glide planes, introduction to space groups.

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

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

UNIT 4: Solid State – II (9hrs)

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

Unit 5: Statistical Thermodynamics- I (9hrs)

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

Unit 6: Statistical Thermodynamics- II (9hrs)

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

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

Reference:

For Units 1-4

1. D. R. Crow, *Principles and Applications of Electrochemistry*, Chapman and Hall London,1979.
2. J.O.M. Bockris and A.K.N. Reddy, *Modern Electrochemistry, Vol. I and II*, Kluwer Academic / Plenum Publishers,2000.
3. Carl. H. Hamann, A. Hamnett, W.Vielstich, *Electrochemistry 2nd edn*., Wiley- VCH,2007.
4. Philip H Reiger, *Electrochemistry 2nd edn*., Chapman & Hall,1994.
5. Praveen Tyagi, *Electrochemistry*, Discovery Publishing House,2006.
6. D.A. McInnes, *The Principles of Electrochemistry*, Dover publications,1961.
7. L.V. Azaroff, *Introduction to Solids*, McGraw Hill, NY,1960.
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.*, Oxford Uty. 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*, AddisonWesley.
3. K. Huary, *Statistical mechanics, Thermodynamics and Kinetics* , JohnWiley.

4. O.K.Rice, *Statistical mechanics*, *Thermodynamics and Kinetics*, Freeman andCo.
5. F.C. Andrews, *Equilibrium statistical mechanics* , John Wiley and sons,1963.
6. M.C. Guptha, *Statistical Thermodynamics* , Wiley eastern Ltd.,1993.

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY
M.Sc. CHEMISTRY – SEMESTER I & II
CHE1L01 & CHE2L04 – INORGANIC CHEMISTRY PRACTICALS– I & II
(3 Credits)

Sl No	Course Outcome	POs/ PSOs	CL	KC
1	To apply the principles of solubility product and common-ion effect to separate and identify cations in the given mixture.	PSO VI	Ap	P
2	To appreciate the different types of volumetric methods for the quantitative analysis of metal ions. the amount of ions by complex metric titrations	PSO VI	U	C
3	To apply the basic principles of Colorimetry for the quantitative analysis of metal ions.	PSO V	Ap	P

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 spottests.

UNIT 2: Volumetric Analysis

Volumetric Determinations using:

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

(b) Cerimetry (Fe^{2+},nitrite)

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

UNIT 3: Colorimetric Analysis

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

References

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

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

M.Sc. CHEMISTRY – SEMESTER I &II

CHE1L02 & CHE2L05 – ORGANIC CHEMISTRY PRACTICALS– I & II

(3 Credits)

Sl No	**Course Outcome**	POs/ PSOs	CL	KC
1	To appreciate the different methods for the purification and separation of organic compounds.	PSO VI	U	C
2	To formulate and perform the different methods for the separation of organic binary mixtures.	PSO VI	Ap	P
3	To perform two stage and three stage organic preparations	PSO V	Ap	P

Unit 1: Laboratory Techniques

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

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

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

Unit 3: Organic preparations-double stage (minimum six) 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, Fuson andCartin, *Systematic Identification of Organic Compounds*, 1964.
3. Fieser, *Experiments in Organic Chemistry*,1957.
4. Dey, Sitaraman and Govindachari, *A Laboratory Manual of Organic*

Chemistry, 3rd Edition,1957.

5. P.R. Singh, D.C. Gupta and K.S. Bajpal, *Experimental Organic Chemistry*, Vol. I and II,1980.
6. Vishnoi, *Practical OrganicChemistry*.
7. Pavia, Kriz, Lampman, and Engel, *A Microscale Approach to Organic Laboratory Techniques,* 5/e, Cengage,2013.
8. Mohrig, Hammond and Schatz, *Techniques in Organic Chemistry: Miniscale, Standard Taper Microscale and Williamson Microscale,* 3/e, W. H. Freeman andCo.,2024

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

M.Sc. CHEMISTRY – SEMESTER I & II

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

Sl No	**Course Outcome**	POs/ PSOs	CL	KC
1	To determine heat of the solution using thermodynamic methods.	PSO V	Ap	P
2	To gain an insight into the phase diagram of eutectic, binary systems.	PSO VI	U	C
3	To apply the principles of viscosity to determine the molecular weight of polymers..	PSO V	Ap	P
4	To perform refractometric analysis, different types of potentiometric and conductometrric titrations.	PSO VI	Ap	P

SECTION A

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

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

Unit 2: Phase Equilibria (minimum 3 experiments)

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

Unit 3: Viscosity (minimum 2 experiments)

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

Unit 4: Distribution Law (minimum 3 experiments)

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

SECTION B

Unit 5: Refractometry (minimum 3 experiments)

1. Determination of molar refractions of pure liquids (e.g.,
water, methanol, ethanol, chloroform, carbon
tetrachloride,glycerol)
2. Determination of composition of liquid mixtures (e.g., alcohol,water, glycerol-water)
3. Determination of molar refraction and refractive index of a solid

Unit 6: Conductivity (minimum 4 experiments)

1. Determination of equivalent conductance of a weak electrolyte(e.g.,
acetic acid), verification of Ostwald's dilution law and calculation of dissociation constant.
2. Determination of solubility product of a sparingly soluble salt (e.g., AgCl,$BaSO_4$)
3. Conductometric titrations
(a) HCl vs NaOH
(b) (HCl + CH_3-COOH) vs NaOH
4. Determination of the degree of hydrolysis of anilinehydrochloride

Unit 7: Potentiometry (minimum 3 experiments)

1. Potentiometric titration: HCl vs NaOH, CH_3-COOH vsNaOH
2. Redox titration: KI vs $KMnO_4$, $FeSO_4$vs$K_2Cr_2O_7$
3. Determination of dissociation constant of acetic acid by potentiometrictitration
4. Determination of pH of weak acid usingPotentiometry
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*, McGrawHill.

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

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

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

CHE3C09 - MOLECULAR SPECTROSCOPY (4 Credits,72hrs)

COURSE OUTCOME

COURSE: MOLECULAR SPECTROSCOPY
COURSE CODE: CHE3C09
Credits: 4 Total hours: 72

	Course outcome	POs/ PSOs	CL	KC
1	Explain the fundamental principles of microwave spectroscopy and interpret its applications in molecular structure determination.	PSO I	U	C
2	Analyze the vibrational spectra of polyatomic molecules and interpret the spectral features.	PSO II	An	P
3	Compare and evaluate the classical and quantum theories of the Raman effect.	PSO I	C	C
4	Explain and evaluate Kramers' theorem and its significance in ESR spectroscopy.	PSO I	E	P
5	Analyze and interpret the Nuclear Overhauser Effect (NOE) in FT-NMR spectroscopy.	PSO I	An	P
6	Explain the principles of Mössbauer spectroscopy and evaluate its applications in chemical and structural studies.	PSO I	U	C
7	Determine and analyze the structures of organic compounds using spectrometric techniques.	PSO II	An	P
8	Explain the principles of Electron Impact Mass Spectrometry (EI-MS) and interpret the resulting mass spectra.	PSO I	U	C

Total hours of instruction 72

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A))**

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

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

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

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

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 (basicsonly).

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* (9hrs)

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* (9hrs)

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 (9hrs)

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

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

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

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

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

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

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

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

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

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

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

References: For Units 1, 2, 3 & 4

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

Chemistry,2/e,

– John Wiley

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

For Units 5, 6, 7 & 8

1. Lambert, Organic Structural Spectroscopy,2/e,—Pearson
2. Silverstein, Spectrometric Identification of Organic Compounds, 6/e,—JohnWiley
3. Pavia, Spectroscopy, 4/e, –Cengage
4. Jag Mohan, Organic Spectroscopy: Principles and Applications,2/e,—Narosa
5. Fleming, Spectroscopic Methods in Organic Chemistry, 6/e, —McGraw-Hill
6. P S Kalsi, Spectroscopy of organic compounds, New Age International,2007
   William Kemp, Organic Spectroscopy**, 3e,** Palgrave,2010

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

CHE3C10 - ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY
(4 Credits, 72h)

COURSE OUTCOME

COURSE: ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY
COURSE CODE: CHE3C10
Credits: 4
Total hours: 72

	Course outcome	POs / PSOs	CL	KC
1	Apply and evaluate the 18-electron and 16-electron rules using the neutral atom method and oxidation state method.	PSO I	E	F
2	Analyze the synthesis, structure, bonding, and reactions of metal carbonyl, nitrosyl, dihydrogen, and dinitrogen complexes.	PSO II	U	C
3	Analyze the structure, bonding, and reactivity of organometallic compounds containing linear and cyclic π-systems.	PSO I	U	C
4	Explain and analyze oxidative addition, reductive elimination, and insertion reactions in organometallic chemistry.	PSO II	U	C
5	Compare and evaluate homogeneous and heterogeneous catalysis involving organometallic compounds.	PSO II	E	C
6	Analyze metal–metal bonding and the structure of metal clusters.	PSO I	An	C
7	Explain the mechanism of oxygen transport by heme proteins.	PSO II	An	P
8	Explain and evaluate the functions of metalloenzymes and electron-carrier metalloproteins in biological systems.	PSO I	U	F

Total hours of instruction 72

Unit 1: Introduction to Organometallic Chemistry (12hrs)

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

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

Unit 2: Organometallic Compounds of Linear and Cyclic π-Systems (12hrs)

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

Unit 3: Organometallic Reactions and Catalysis (12hrs)

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 (12hrs)

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 (12hrs)

Metallo enzymes and electron carrier metallo proteins. Iron enzymes: Cytochrome P-450, catalase and peroxidase.Copper enzymes: Oxidase, superoxide dismutase and tyrosinase. Lewis acid role of Zn(II) and Mn(II) containing enzymes. Carboxypeptidase. Vitamin B_{12} and coenzymes.Chlorophil II- Photosystem I and II. Nitrogen fixation-Nitrogenases. Anticancer drugs.

References:

1. N.N. Greenwood and A.Earnshaw, *Chemistry of Elements,* 2/e, Elsevier Butterworth-Heinemann,2005.
2. J.E.Huheey, E.A.Keiter, R.L.Keiter. O.K.Medhi, *Inorganic Chemistry, principles of structure and reactivity,* Pearson Education,2006.
3. G.L.Miessler, D.A.Tarr, *Inorganic Chemistry,* Pearson,2010.
4. D.F.Shriver, P.W.Atkins, *Inorganic Chemistry,* Oxford University Press,2002
5. William W Porterfield, *Inorganic Chemistry-A unified approach,* Academic Press,2005.
6. Keith F Purcell, John C Kotz, *Inorganic Chemistry,* Cengage Learning,2010.
7. James E House, *Inorganic Chemistry,* Academic Press,2008.
8. B.Douglas, D.McDaniel, J.Alexander, *Concepts and Models of Inorganic Chemistry,* Wiley Student Edition,2006.
9. F.A.Cotton and G.Wilkinson, *Advanced Inorganic Chemistry*,Wiley.

10. R.C.Mehrothra and A.Singh, *Organometallic Chemistry, A Unified Approach, W*ileyEastern.
11. P.Powell, *Principles of Organometallic Chemistry,ELBS.*
12. B.D.Gupta and A.J.Elias, *Basic Organometallic Chemistry, Concepts, Synthesis and Applications*, Universities Press,2010.
13. Piet W.N. M.van Leeuwen, *Homogeneous Catalysis*, Springer,2010.S.J. Lippard and J.M.Berg, *Principles of Bioinorganic Chemistry*, University ScienceBooks.
14. I. Bertini, H.B. Grey, S.J. Lippard and J.S.Valentine, *Bioinorganic Chemistry, Viva Books Pvt. Ltd.,1998.*

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

COURSE OUTCOME

COURSE: REAGENTS &TRANSFORMATIONS IN ORGANIC CHEMISTRY
COURSE CODE: CHE3C11
Credits: 4
Total hours: 72

	Course outcome	POs / PSOs	CL	KC
1	Explain and apply various oxidation methods in organic synthesis.	PSO I	U	C
2	Analyze and evaluate synthetic reagents used in organic transformations.	PSO I	An	C
3	Explain and apply various reduction methods in organic synthesis.	PSO I	S	C
4	Classify and analyze polymers based on their structure, properties, and applications.	PSO II	An	C
5	Analyze the structure, synthesis, and reactions of heterocyclic compounds.	PSO II	S	C
6	Explain and evaluate molecular rearrangements and transformations in organic reactions.	PSO I	U	C
7	Analyze the mechanisms of various rearrangement reactions and predict their products.	PSO II	S	P
8	Apply the concepts and terminology of supramolecular chemistry to explain molecular recognition and self-assembly processes.	PSO II	U	P

Total hours of instruction 72

(Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A),Study (S))

Unit 1: Oxidations (12 hrs)

Oxidation of alcohols to carbonyls using DMSO, oxoammonium ions and transition metal oxidants (chromium, manganese, iron, ruthenium). Epoxydation of alkenes by peroxy acids, Sharpless asymmetric epoxidation, Jacobsen epoxidation, dihydroxylation of alkenes using permanganate ion and osmium tetroxide, Prévost and Woodward dihydroxylations, Sharpless asymmetric dihydroxylation. Allylic oxidation with CrO_3-Pyridine reagent. Oxidative cleavage of alkenes to carbonyls using O_3. Oxidative decarboxylation, Riley reaction, Baeyer-Villiger oxidation, Dess- Martin oxidation, Swern oxidation, hydroboration-oxidation.

Unit 2: Reductions (12 hrs)

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

Unit 3: Synthetic Reagents (12 hrs)

Synthetic applications of Crown ethers, β-cyclodextrins, PTC, ionic liquids, Baker's yeast, NBS, LDA, $LiAlH_4$, $LiBH_4$, DIEA, BuLi, diborane, 9-BBN, t-butoxycarbonylchloride, DCC, Gilman's reagent, lithium dimethyl cuprate, tri-n-butyltinhydride, 1,3-dithiane, trimethyl silyl chloride, $Pb(OAc)_4$, ceric ammonium nitrate, DABCO, DMAP, DBU, DDQ, DEAD and Lindlar catalyst in organic synthesis.

Unit 4: Chemistry of Polymers (12 hrs)

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

Natural and synthetic rubbers.

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

Unit 5: Heterocyclic chemistry and supramolecular chemistry (12 hrs)

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

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

Unit 6: Molecular Rearrangements and Transformations (12 hrs)

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

References:

1. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press,2011.
2. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis,* 3/e, CRC Press,1998.
3. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4/e, Cambridge UniversityPress.
4. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, Part B, 5/e, Springer,2007.
5. M. B. Smith, J. March, *March's Advanced Organic Chemistry*, 6/e, John Wiley & Sons, 2007.
6. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 2/e, Oxford University Press, 2012.
7. J. J. Li, *Name Reactions*, 4/e, Springer,2009.
8. V. K. Ahluwalia and R. Aggarwal, *Organic Synthesis: Special Techniques*, 2/e, Narosa

Publishing House,2006.

9. G. Odiyan, *Principles of Polymerisation*, 4/e, Wiley,2004.
10. V.R. Gowariker and Others, *Polymer Science*, Wiley EasternLtd.
11. I.L. Finar, *Organic Chemistry*, Vol. II, 5/e, ELBS,1975.
12. J. A. Joules and K. Mills, *Heterocyclic Chemistry*, 4/e, Oxford University Press,2004.
13. T. L. Gilchrist, *Heterocyclic Chemistry*, 3/e, Pearson,1997.
14. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3/e Addison-Wesley,1998.
15. F. Vogtle, *Supramolecular Chemistry*, John Wiley & Sons, Chichester,1991.
16. J.M.Lehn, *Supramolecular Chemistry*,VCH.

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

M.Sc. CHEMISTRY (CBCSS PATTERN) - SEMESTER III
SYNTHETIC ORGANIC CHEMISTRY (ELECTIVE) (4 Credits, 72hrs)
COURSE OUTCOME

COURSE: SYNTHETIC ORGANIC CHEMISTRY
COURSE CODE: CHE3E01
Credit :4
Total hours: 72

	Course outcome	POs/ PSOs	CL	KC
1	Explain and apply reagents used for oxidation and reduction reactions in organic synthesis.	PSO I	U	C
2	Analyze and compare homogeneous and heterogeneous catalytic hydrogenation processes.	PSO I	An	C
3	Evaluate the synthetic applications of organometallic and organo-nonmetallic reagents in organic transformations.	PSO II	E	C
4	Analyze the chemistry and reactivity of carbonyl compounds and predict their reaction outcomes.	PSO I	U	F
5	Analyze the mechanisms and synthetic applications of coupling reactions.	PSO II	S	P
6	Evaluate methods employed in multistep organic synthesis and select appropriate synthetic strategies.	PSO II	E	P
7	Apply the principles of retrosynthetic analysis to design synthetic routes for organic molecules.	PSO II	An	P
8	Explain and apply the concepts of phase-transfer catalysis in organic reactions.	PSO I	U	C

Total hours of instruction 72

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A),Study (S))**

Unit 1: Reagents for Oxidation and Reduction (12hrs)

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

Catalytic hydrogenations (heterogeneous and homogeneous), metal hydrides, Birch reduction, hydrazine and diimide reduction.

Unit 2: Organometallic and Organo-nonmetallic Reagents (12hrs)

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

Unit 3: Chemistry of Carbonyl Compounds (12hrs)

Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides, amides. Substitution at α-carbon, aldol and related reactions, Claisen, Darzen, Dieckmann, Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Reaction with phosphorous and sulfurylides.

Protecting groups, functional group equivalents, reversal of reactivity (Umpolung), Introduction to combinatorial chemistry.

Unit- 4. Coupling Reactions (12hrs)

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

Unit 5: Multi step Synthesis (12hrs)

Multi step Synthesis**:** Synthetic analysis and planning, Target selection, Elements of a Synthesis (Reaction methods, reagents, catalysts, solvents, protective groups for hydroxyl, amino, Carbonyl and carboxylic acids, activating groups, leaving groups synthesis and synthetic equivalents. Types of selectivities (Chemo, regio, stereo selectivities) synthetic planning illustrated by simple molecules, disconnections and functional group interconversions, uplong reactions and use in synthesis, Introduction to retrosynthetic analysis, Synthesis of longifolene, Corey lactone, Djerassi Prelog lactone

Unit 6: Retro Synthetic Analysis and Heterocyclics (12hrs)

Retrosynthesis: General principles of retrosynthetic analysis - synthons and reagents, donor and acceptor synthons, umpolung, protecting group chemistry and functional group interconversions. One group and two group C - X and C - C disconnections, functional group transposition. Examples for a few retrosynthetic analyses - paracetamol from phenol, benzocain from toluene and propranolol from 1 - naphthol.

Structure, synthesis and reactions of fused ring heterocycles: Benzofuran, Indole, Benzothiophene, Quinoline, Benzoxazole, Benzthiazole, Benzimidazole, Triazoles , Oxadiazoles and Tetrazole.

Structure and synthesis of Azepines, Oxepines, Thiepins, Diazepines and Benzodiazepines

Structure and synthesis (Reichstein process) of Vitamin C (Reichstein process).

References:

1. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press,2011.
2. S. Warren and P. Wyatt, *Organic Synthesis: Strategy and Control*, JohnWiley
3. S. Warren: *Organic Synthesis: The Disconnection Approach*, JohnWiley
4. H. O. House: *Modern Synthetic Reactions*, W. A.Benjamin
5. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4/e, Cambridge UniversityPress.
6. T. W. Greene and P. G. M. Wuts: *Protecting Groups in Organic Synthesis*, 2nd ed., JohnWiley
7. MBSmithandJ.March:*AdvancedOrganicChemistry-Reactions,MechanismsandStructure*,

6th ed., John Wiley

8. T. H. Lowry and K. S. Richardson: *Mechanism and Theory in Organic Chemistry*, 3rded.
9. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry*, Part A and B, 5/e, Springer, 2007
10. A. Pross: *Theoretical and Physical Principles of Organic Chemistry*, JohnWiley
11. T.W. Graham Solomons: *Fundamentals of Organic Chemistry*, 5th ed., JohnWiley
12. I. L. Finar: *Organic Chemistry* Volumes 1 (6th ed.),Pearson
13. J. Clayden, N. Green, S. Warren and P. Wothers: *Organic Chemistry*, 2/e, Oxford University Press
14. J. J. Li, *Name Reactions*, 4/e, Springer,2009.
15. N. K. Terret: *Combinatorial Chemistry*, Oxford University Press,1998.

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

CHE3E02 - COMPUTATIONAL CHEMISTRY (ELECTIVE) (4credits, 72 hrs)

	Course outcome	POs/ PSOs	CL	KC
1	Explain and classify computational chemistry methods and analyze the need for approximate methods in chemical calculations.	PSO I	U	C
2	Apply molecular dynamics and Monte Carlo methods to calculate thermodynamic properties, analyze simulation results, and estimate associated errors.	PSO I	Ap	P
3	Perform molecular dynamics and Monte Carlo simulations using continuous potentials and random number generators, and analyze the resulting data.	PSO II	Ap	P
4	Analyze Hartree–Fock methods, perform self-consistent field (SCF) calculations for polyatomic molecules, and evaluate electron correlation methods.	PSO I	An	P
5	Compare and evaluate Density Functional Theory (DFT) and Hartree–Fock methods, including the application of exchange–correlation functionals.	PSO II	U	C
6	Evaluate and select appropriate basis sets for quantum chemical calculations based on computational efficiency and accuracy requirements.	PSO II	E	P

Total hours of instruction 72

(Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C), Evaluate (E),Analyse (A), Apply (Ap))

Unit 1: Introduction to Computational Chemistry (12 hrs)

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 (12 hrs)

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 (12 hrs)

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 (12 hrs)

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 (12 hrs)

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

UNIT 6: Basis Set Approximation (12 hrs)

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 cputime.

References:

1. C. J. Cramer, *Essentials of computational Chemistry: Theories and models*, John Wiley & Sons 2002.
2. Frank Jensen, *Introduction to Computational Chemistry*, John Wiley & Sons LTD1999.
3. J. Foresman & Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.
4. David Young, *Computational Chemistry- A Practical Guide for Applying Techniques to Real- World Problems"*, Wiley -Interscience,2001.
5. Errol G. Lewars, *Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics*, 2 nd edn., Springer2011.
6. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc.,2009.
7. P.W. Atkins & R.S. Friedman, *Molecular quantum mechanics*, 4th Edition, Oxford University Press,2005.
8. W. Koch, M.C. Holthausen, *"A Chemist's Guide to Density Functional Theory"*, Wiley- VCH Verlag2000

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

CHE3E03- GREEN CHEMISTRY AND NANOCHEMISTRY (ELECTIVE)

(4credits, 72 hrs)

COURSE OUTCOME

COURSE: GREEN CHEMISTRY AND NANOCHEMISTRY (ELECTIVE)
COURSE CODE CHE3E03
Credits: 4

Total hours: 72

	Course outcome	POs/ PSOs	CL	KC
1	Explain and evaluate the goals, principles, and methodologies of green chemistry and apply appropriate tools for sustainable chemical practices.	PSO VII	U	C
2	Apply microwave activation techniques to perform organic reactions and analyze the effects and advantages of microwave irradiation.	PSO I	Ap	P
3	Apply and evaluate alternative synthetic methods, reagents, and reaction conditions, including ionic liquids, phase-transfer catalysts, and supercritical carbon dioxide, for green chemistry applications.	PSO V	Ap	P
4	Explain the properties, classification, and synthesis of nanomaterials and apply suitable methods for the preparation of inorganic and organic nanomaterials.	PSO II	U	P
5	Employ and interpret advanced characterization techniques such as AFM, TEM, STEM, STM, SNOM, and surface plasmon spectroscopy for the analysis of nanoscale materials.	PSO VI	Ap	P
6	Analyze the structure, properties, and synthesis of carbon clusters and nanostructures, including fullerenes and carbon nanotubes, and evaluate their applications in various fields.	PSO V	U	C

Total hours of instruction 72

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E))**

Unit I: Introduction to green chemistry (12hrs)

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

UNIT-2: Microwave mediated organic synthesis (MAOS) (12hrs)

Microwave activation –advantage of microwave exposure – specific effects of microwave – Neat reactions – solid supports reactions _ Functional group transformations – condensations reactions

– oxidations – reductions reactions – multi-componentreactions.

Unit 3: Alternative synthesis, reagents and reaction conditions (12hrs)

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

Unit 4: Nanomaterials – An Introduction & Synthetic Methods (12hrs)

Definition of nanodimensional materials - Historical milestones - unique properties due to nanosize,Quantum dots, Classification of Nanomaterials .General methods of synthesis of nanomaterials – Hydrothermal synthesis,Solvothermal synthesis,Microwave irradiation, sol – gel and Precipitation technologies, Combustion Flame-Chemical Vapor Condensation Process, gas Phase Condensation Synthesis,Reverse Micelle Synthesis, Polymer – Mediated Synthesis, Protein Microtube – Mediated SynthesisSynthesis of Nanomaterials using microorganisms and other biological agents, Sonochemical Synthesis, Hydrodynamic Cavitation.Inorganicnanomaterials – Typical examples –nano TiO2 / ZnO/CdO/CdS , Organic nanomaterials – examples – Rotaxanes and Catenanes

Unit 5: Techniques for Characterisation of nanoscale materials (12hrs)

Principles of Atomic force microscopy (AFM)- Transmission electron microscopy (TEM)- Resolution and scanning transition electron microscopy (STEM) Scanning Tunneling Microscopy (STM) Scanning nearfield optical microscopy (SNOM),Scanning ionconductance microscope, scanning thermal microscope, scanning probe microscopes and surface plasmon spectroscopy.

Unit 6: Carbon Clusters and Nanostructures (12hrs)

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

References:

For Units 1, 2 & 3

- V. K. Ahluwalia, *Green Chemistry – Environmentally benign reactions,* Ane Books India (Publisher),(2006).
- V. K. Ahluwalia, *Green Chemistry : A Textbook*, Narosa Publishing House,2013.
- *Green Chemistry – Designing Chemistry for the Environment* – edited by Paul T. Anastas & Tracy C. Williamson. Second Edition,(1998).
- *GreenChemistry–Frontiersinbenignchemicalsynthesisandprocesses*-editedbyPaul T. Anastas & Tracy C. Williamson. Oxford University Press, (1998).
- *Green Chemistry – Environment friendly alternatives*- edited by Rashmi Sanghi & M. M. Srivastava, Narora Publishing House,(2003).

For Units 4, 5 & 6

1. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), *The Chemistry of Nanomaterials*, Vol.1, 2, Wiley –VCH, Weinheim,2004.
2. C.P. Poole, Jr:
3. F.J. Owens, *Introduction to Nanotechnology* Wiley Interscience, New Jersey, 2003
4. Kenneth J. Klabunde (Ed), *Nanoscale materials in Chemistry*, Wiley- Interscience, New York, 2001.
5. T. Pradeep, *Nano: The Essentials in understanding nanoscience and nanotechnology*, Tata McGraw Hill, New Delhi,2007.

6. H. Fujita (Ed.), *Micro machines as tools in nanotechnology*, Springer- Verlag, Berlin,2003.
7. Bengt Nolting, *Methods in modern biophysics*, Springer-Verlarg, Berlin, First Indian Reprint, 2004. (Pages 102-146 for Unit II and 147 – 163 for UnitV)
8. H. Gleiter, *Nanostructured Materials: Basic Concepts, Microstructure and Properties*
9. W. Kain and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, John-Wiley R Sons, NewYork.
10. T. Tang and p. Sheng (Eds), *Nano Science and Technology Novel Structures andPhenomena*, Taylor & Francis, New York, 2004.
11. A. Nabok, *Organic and Inorganic Nanostructures*, Artech House, Boston,2005.
12. Edward A. Rietman, *Molecular engineering of Nanosystems*, Springer- Verlag, New York, 2001.
13. Home page of Prof. Ned Seeman -http://seemanlab4.chem.nyu.edu/
14. Nano letters - http://pubs.acs.org/journals/nalefd/index.html
    Nanotation -http://www.acsnanotation.org/

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

M.Sc. CHEMISTRY (CBCSS PATTERN) - SEMESTER IV CHE4C12-

INSTRUMENTAL METHODS OF ANALYSIS (4 Credits,72 Hrs)

COURSE OUTCOME

COURSE: INSTRUMENTAL METHODS OF ANALYSIS
COURSE CODE CHE4C12
Credits: 4
Total hours: 72
4hrs/week

	Course outcome	POs/ PSOs	CL	KC
1	Apply statistical methods to analyze experimental data and estimate errors in analytical measurements.	PSO I	U	P
2	Explain and apply the principles of gravimetric analysis using inorganic precipitating agents such as NH_3, H_2S, $(NH_4)_2MoO_4$, and NH_4SCN.	PSO III	Ap	M
3	Explain and evaluate neutron activation analysis for qualitative and quantitative chemical analysis.	PSO I	Ap	C
4	Analyze the capabilities and limitations of optical instrumental methods in chemical analysis.	PSO II	U	P
5	Explain the components and interpret the principles of operation of analytical instruments.	PSO I	Ap	M
6	Analyze chromatographic methods, detectors, and CHN analysis using gas chromatography.	PSO I	U	C
7	Explain and interpret thermogravimetric analysis (TGA), differential thermal analysis (DTA), differential scanning calorimetry (DSC), and their instrumentation.	PSO I	U	C
8	Explain and compare amperometry, coulometry, chronopotentiometry, and anodic stripping voltammetry and their analytical applications.	PSO I	U	C

Total hours of instruction	70	2

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A),Apply (Ap) ,Metacognitive Knowledge(M))**

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

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 (9hrs)**

Gravimetry: **s**olubility product and properties of precipitates-nucleation, growth and aging, co-precipitation and post precipitation, drying and ignition. Inorganic precipitating agents: NH_3, H_2S, H_2SO_4, $(NH_4)_2MoO_4$ andNH_4SCN.

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

Acid-Base and precipitation titrations: theory of neutralisation titrations, indicators for acid/base titrations, titration curves of strong acid, strong base, weak acid, weak base and polyprotic acids. Buffer solutions.

Titrations in nonaqueous media. Different solvents and their selection for a titration. Indicators for non-aqueoustitrations

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, alkali metric and exchange reactions), masking and demasking agents, selective demasking, metal ion indicators - murexide, eriochrome black T, Patton and Reeder's indicators, bromo pyro gallol red, xylenol orange, variamine blue.

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

Potentiometry: techniques based on potential measurements, direct potentiometric systems different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, modern modifications, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, bio membrane, biological and bio catalytic electrodes

, importance of selectivity coefficients. Polarography micro electrode and their specialities, potential and current variations at the micro electrode systems, conventional techniques for concentration determination, limitations of detection at lower concentrations, techniques of improving detection limit-rapid scan, ac, pulse, differential pulse square wave polarographic techniques. Applications of polarography.

Unit 4 Electro Analytical Methods II (9hrs)

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

Unit5 Optical Methods - I (9hrs)

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

Unit 6 Optical Methods - II (9 hrs)

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

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

Thermogravimetry(TG), Differential Thermal Analysis(DTA) and Differential Scanning Calorimetry(DSC) and their instrumentation. Thermometric Titrations.

Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications. Principle and applications of isotope dilution methods.

Unit 8: Chromatography (9 hrs)

Chromatography-classification-column-paper and thin layer chromatography. HPLC-outline study of instrument modules. Ion – exchange chromatography-Theory. Important applications of chromatographic techniques. Gel 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 AnalyticalChemistry,*
3. 9th Edn., Cengage Learning., 2014.
4. J.G. Dick, *Analytical Chemistry*, R.E. KriegerPub.,1978.50
5. J.H. Kennedy, *Analytical Chemistry: Principles*, Saunders College Pub.,1990.
6. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, *Vogel's Text Book of Quantitative Chemical Analysis*, 5th Edn., John Wiley&sons,1989.
7. C.L. Wilson, D.W. Wilson, *Comprehensive Analytical Chemistry*, Elsevier,1982.
8. G.D. Christian, J.E. O'Reilly, *Instrumental Analysis*, Allyn & Bacon,1986.
9. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall,1967.
10. A.I. Vogel, *A Textbook of Practical Organic Chemistry*, 5/e Pearson,1989.
11. H.A. Laitinen, W.E. Harris, *Chemical Analysis*, McGrawHill,1975.
12. V.K. Ahluwalia, *Green Chemistry: Environmentally Benign Reactions*, CRC,2008.
13. F.W. Fifield, D. Kealey, *Principles and Practice of Analytical Chemistry,* Blackwell Science,2000.
14. G.Gringauz, *Introduction to Medical Chemistry,* Wiley-VCH,1997.
15. Harkishan Singh and V.K.Kapoor, *Medicinal and Pharmaceutical Chemistry,* Vallabh Prakashan,2008.
16. W.Bannwarth and B.Hinzen, *Combinatorial Chemistry-From Theory to Application,2nd*
17. Edition, Wiley-VCH, 2006.
18. A.W.Czarnik and S.H.DeWitt, *A Practical Guide to Combinatorial Chemistry,* 1st
19. Bansal N K, Kleeman M and Mells M, *Renewable Energy Sources and Conversion Technology,* Tata McGraw-Hill.(1990)

20. Kothari D.P., *"Renewable energy resources and emerging technologies",* Prentice Hall of India Pvt. Ltd.,2008.
21. Rai G.D, *"Non-Conventional energy Sources"*, Khanna Publishers,2000.
22. Michael Grätzel, *J. Photochemistry and Photobiology C: Photochemistry Reviews* 4 (2003) 145–153, *Solar Energy Conversion by Dye-Sensitized Photovoltaic Cells*, Inorg. Chem., Vol. 44, No. 20, 20056841-6851.
23. Yoshihiro Hamakawa,Thin-Film Solar Cells-Next *Generation Photovoltaics and Its Applications*, Springer Series in Photonics 13,2004

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

CHE4E04 - PETROCHEMICALS AND COSMETICS (ELECTIVE)
(4Credits, 72hrs)

COURSE OUTCOME

COURSE: PETROCHEMICALS AND COSMETICS (ELECTIVE)
COURSE CODE CHE4E04
Credits: 4
Total hours: 72
4hrs/week

	Course outcome	POs/ PSOs	CL	KC
1	Evaluate the importance and applications of reforming processes in the production of gasoline and petrochemicals.	PSO I	E	P
2	Analyze the industrial uses and applications of various hydrocarbons derived from petroleum.	PSO III	Ap	P
3	Evaluate the significance and industrial applications of important organic compounds derived from petroleum.	PSO VII	Ap	C
4	Analyze the composition of crude petroleum and interpret the physical properties and test methods used for petroleum and its derivatives.	PSO II	U	M
5	Evaluate the processes and equipment employed in the treatment and processing of residual liquids obtained from petroleum distillation.	PSO I	U	C
6	Explain and analyze the industrial applications and uses of various petroleum products.	PSO II	U	C
7	Evaluate the effectiveness and applications of purification techniques used in petroleum refining processes.	PSO VI	Ap	M
8	Prepare and analyze cosmetic formulations and evaluate their chemical composition and functional properties.	PSO III	U	P

Total hours of instruction	72	2

(Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A),Apply (Ap) ,Metacognitive Knowledge(M))

Unit 1: Introduction to Petrochemistry (9hrs)

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 (9hrs)

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 (9hrs)

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 (9hrs)

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 inter facial tensions.

4.RefractiveIndex. 5.Flash and fire points .6.Cloudandpourpoints.

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

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Unit 5: Distillation of Crude Petroleum (9hrs)

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 (9hrs)

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 (9hrs)

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 (9hrs)

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 andpetrochemicals*,
3. John W. Hill, *Chemistry for Changing times*, SurjeetPublication
4. Uttam Ray Chaudhuri, *"Fundamentals of Petroleum and PetrochemicalEngineering",* , Boca Raton London New York.
5. S ukumar Maiti, *"Introduction To Petrochemicals"* India Book House PvtLtd.
6. Gabriella Baki, Kenneth S. Alexander, *"Introduction to Cosmetic Formulation and Technology",*Wiley.
7. Tony Curtis, David Williams, *"Introduction to Perfumery",* Micelle Press; 2ndedition

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

CHE4E05 - INDUSTRIAL CATALYSIS (ELECTIVE (4 Credits, 72hrs)

COURSE OUTCOME

COURSE: INDUSTRIAL CATALYSIS
COURSE CODE: CHE4E05
Credits: 4
Total hours: 72
4hrs/week

	Course outcome	POs / PS Os	CL	KC
1	Compare and differentiate physisorption and chemisorption based on their mechanisms and characteristics.	PSO I	U	P
2	Analyze and evaluate the kinetics of heterogeneous catalytic reactions.	PSO I	E	C
3	Explain and apply Langmuir, BET, and Freundlich adsorption isotherms to adsorption phenomena.	PSO II	U	P
4	Analyze the methods used for the preparation and deactivation of catalysts.	PSO I	An	P
5	Explain and apply the principles of phase-transfer catalyzed reactions.	PSO I	U	F
6	Explain and evaluate biocatalysts and their immobilization techniques.	PSO I	U	F
7	Analyze and evaluate catalysts employed for environmental protection and pollution control.	PS O III	E	F
8	Explain and evaluate the role of heterogeneous catalysts in industrial and environmental processes.	PSO I	U	F

Total hours of instruction 72

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A))**

Unit 1: Introduction to Adsorption process (9hrs)

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 chemisorption – activated and non-activated chemisorption – absolute rate theory – electronic theories, hysteresis and shapes of capillaries.

Unit 2: Kinetics and Catalysis (9hrs)

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,*“Introductiontoprinciplesofheterogeneouscatalysis”,* 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 - Praparative Methods(9hrs)

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 ofzeolites, mechanism of nuclear formation and crystal growth, structuresof some selected zeolites – zeolites A, X and Y, pentasils – ZSM-5, ZSM-11, shape selective catalysis by zeolites.

Unit 4: Deactivation of Catalysts (9hrs)

Deactivation of catalysts, classification of catalyst deactivation processes, poisoning of catalysts, coke formation on catalysts, metal deposition on catalysts, sintering of catalysts, Regeneration of deactivated catalysts, feasibility of regeneration, description of coke deposit and kinetics of regeneration.

References:

1. J.R. Anderson and M. Boudart (Eds), *"Catalysis, Science and Technology",* Vol 6, Springer- Verlag, Berlin Heildberg,1984.
2. R.B. Anderson, *"Experimental methods in catalysis research",* Vol I, II, Academic press, NY,1981.
3. R. Szostak, *"Molecular sieves: principles of synthesis and identification*", Van Nostrand, NY, 1989.
4. R. Hughes, *"Deactivation of catalysts",* Academic press, London,1984.

UNIT 5: Phase Transfer Catalysis (9hrs)

Basic concepts in phase transfer catalysis – phase transfer catalyzed reactions – basic steps of phase transfer catalysis – effect of reaction variables on transfer and intrinsic rates – outline of compounds used as phase transfer catalysts. Use of quaternary salts – macrocyclic and macrobicyclic ligands – PEG's and related compounds –use of dual phase transfer catalyst or co-catalyst in phase transfer systems –separation and recovery of phase transfer catalysts. Insoluble phase transfer catalysts.

UNIT 6: Biocatalysis (9hrs)

Enzymes – an introduction to enzymes – enzymes as proteins – classification and nomenclature of enzymes – structure of enzymes – how enzymes work – effect on reaction rate – thermodynamic definitions – catalytic power and specificity of enzymes – optimization of weak interactions between enzyme and substrate in the transition state – binding energy, reaction specificity and catalysis – specific catalytic groups contributing to catalysis. Immobilized biocatalysts – definition and classification of immobilized biocatalysts – immobilization of coenzymes.

References:

1. C.M. Starks, C.L. Liotta And M. Halpern, *"Phase Transfer Catalysis – Fundamentals, Applications And Industrial Perspectives"*, Chapman & Hall, New York,1994.
2. A.L. Lehninger, *"Principles of Biochemistry",* Worth Publishers, USA,1987.

UNIT 7: Industrial Catalysis-1 (9hrs)

Oil based chemistry; catalytic reforming; catalytic cracking; paraffin cracking; naphthenic cracking; aromatic hydrocarbon cracking; isomerization; hydrotreatment; hydrodesulphurization; hydrocracking; steam cracking; hydrocarbons from synthesis gas; Fisher-Tropsch process, Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

UNIT 8: Industrial Catalysis-II (9hrs)

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 CatalyticProcesses",* 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

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SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

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

COURSE OUTCOME

COURSE: NATURAL PRODUCTS & POLYMER CHEMISTRY
COURSE CODE: CHE4E06
Credits: 4
Total hours: 72
4hrs/week

	Course outcome	POs/ PSOs	CL	KC
1	Isolate, characterize, and evaluate important constituents of essential oils and oleoresins and analyze their applications in aromatherapy.	PSO I	U	P
2	Explain and analyze the biosynthetic and synthetic pathways of prostaglandins and evaluate their physiological roles.	PSO I	E	C
3	Classify alkaloids based on structure and determine their structures using degradative reactions with reference to quinine, atropine, and related compounds.	PSO II	U	P
4	Compare and analyze natural and synthetic dyes and pigments, including β-carotene, indigo, and cyclic tetrapyrroles.	PSO I	Ap	P
5	Explain and apply the principles of copolymerization and analyze various polymerization techniques such as bulk, solution, suspension, emulsion, and dispersion polymerization.	PSO II	U	M
6	Analyze polymer stereochemistry and evaluate methods used for polymer characterization.	PSO IV	U	P
7	Analyze and evaluate catalysts employed for environmental protection and pollution control.*	PSO III	E	F
8	Explain and evaluate the role of heterogeneous catalysts in industrial and environmental processes.*	PSO I	U	F

Total hours of instruction 72

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A),Apply (Ap) ,Metacognitive Knowledge(M))**

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

Classification of Natural Products**:** Classification of Natural products based on chemical structure, physiological activity, taxonomy and Biogenesis. Carbohydrates, Terpenoids, Carotenoids, alkaloids, steroids, anthocyanins etc. Methods of isolation of each class of compound

Essential Oils:Isolation and study ofimportant constituents of lemon grass oil, citronella oil, cinnamon oil, palmarosa oil, turpentine oil, clove oil, sandalwood oil, Essential oils of turmeric and ginger. Oleoresins of pepper, chilly, ginger and turmeric. Aromatherapy.

UNIT 2: Terpenoids and Steroids (9 hrs)

Terpenoids: classification, structure elucidation and synthesis of abietic acid.

Steroids : Classification, structure of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone.Classification, structure and synthesis of prostaglandins, biosynthesis of fatty acids, prostaglandins, terpenoids andsteroids.

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

UNIT 3: Alkaloids and Anthocyanins (9 hrs)

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

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

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

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

References:

1. M. B. Smith, *Organic Synthesis*, 3/e, Academic Press,2011.
2. F. A. Carey and R. J. Sundberg*: Advanced Organic Chemistry (part B),* 3rd ed., PlenumPress.
3. T.W. G. Solomons: *Fundamentals of Organic Chemistry*, 5th ed., JohnWiley
4. H. O. House: *Modern Synthetic Reactions*, W. A.Benjamin
5. W. Carruthers: *Some Modern Methods of Organic Synthesis*, 4/e, CambridgeUniversity Press.
6. I. L. Finar: *Organic Chemistry* Volumes 1 (6th ed.) and 2 (5th ed.), Pearson.
7. J. Clayden, N. Green, S. Warren and P. Wothers: *Organic Chemistry*, 2/e, OxfordUniversityPress
8. N. R. Krishnaswamy: *Chemistry of Natural Products*; A Unified Approach, UniversitiesPress
9. R. J. Simmonds: *Chemistry of Biomolecules: An Introduction*,RSC
10. R. O. C. Norman: *Principles of Organic Synthesis*, 3rd ed., CRC Press,1998.
11. J. M. Lehn, *SupramolecularChemistry*

UNIT 5: Polymerization Processes (9 hrs)

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

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

Polymer Stereochemistry. Organizational features of polymer chains. Configuration and conformation, Tacticity, Repeating units with more than one asymmetric center. Chiral polymers – main chain and side chain. Stereoregular polymers. Manipulation of polymerization processes. Zeigler-Natta and Kaminsky routes. Coordination polymerization. Metallocene and Metal oxidecatalysts.

Polymer Characterization. Molecular weights. Concept of average molecular weights, Molecular weight distribution. Methods for determining molecular weights. 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 hrs)

Polymer Solutions. Treatment of dilute solution data. Thermodynamics. Flory-Huggins equation. Chain dimension-chain stiffness – End-to-end distance. Conformation-random coil, Solvation and Swelling. Flory-Reiner equation. Determination of degree of crosslinking and molecular weight between crosslinks.

Industrial polymers. Synthesis, Structure and applications. Polyethylene, polypropylene, polystyrene. Homo and Copolymers. Diene rubbers. Vinyl and acrylic polymers. PVC, PVA, PAN, PA. 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 hrs)

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

References:

1. F.W. Billmayer. *Textbook of Polymer* Science. 3rd Edn, Wiley. N.Y.1991.
2. G. Odiyan, *Principles of Polymerisation*, 4/e, Wiley,2004.
3. V.R. Gowriker and Others, *Polymer Science*, Wiley EasternLtd.
4. J.M.G Cowie. *Polymers: Physics and Chemistry of Modern Materials*. Blackie.

London,1992.

5. R.J.Young, *Principles of Polymer Science*, 3rd Edn. , Chapman and Hall. N.Y.1991.
6. P.J. Flory. *A Text Book of Polymer Science.* Cornell University Press. Ithacka,1953.
7. F. Ullrich, *Industrial Polymers*, Kluwer, N.Y.1993.
8. H.G.Elias, *Macromolecules,* Vol. I & II, Academic, N.Y.1991.

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

CHE4E07 - MATERIAL SCIENCE (ELECTIVE) (4 credits, 72hrs)

COURSE OUTCOME

COURSE: - MATERIAL SCIENCE (ELECTIVE)
COURSE CODE: CHE4E06
Credits: 4
Total hours: 72
4hrs/week

	Course outcome	POs/ PSOs	CL	KC
1	Explain and classify engineering materials based on their properties and analyze their mechanical characteristics, including tensile strength and hardness.	PSO I	U	C
2	Analyze the structure and properties of ceramics and predict material behavior using phase diagrams.	PSO I	An	P
3	Apply various synthesis methods for nanomaterials and evaluate their applications in diverse fields.	PSO II	Ap	P
4	Evaluate the properties and applications of ultra-pure materials, ferroelectric materials, piezoelectric materials, and metallic glasses.	PSO I	E	C
5	Explain and evaluate the properties and applications of magnetic materials, superconductors, and high-temperature superconductors.	PSO I	U	C
6	Analyze the properties, production methods, and applications of functional and industrial polymers.	PSO IV	An	C
7	Explain and classify engineering materials based on their properties and analyze their mechanical characteristics, including tensile strength and hardness.	PSO III	A	C
8	Analyze and evaluate fracture mechanics, including microstructural features, Weibull statistics, and creep behavior of materials.	PSO VII	A	C

Total hours of instruction 72

(Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A),Apply (Ap))

Unit 1: Introduction to Material Science (9hrs)

Introduction, classification of materials, functional classification, classification based on structure, environmental and other effects, material design and selection;

Mechanical properties – significance and terminology, the tensile test, true stress and true strain, bend test, hardness of materials.

Unit 2: Ceramic Materials (9hrs)

Definition of ceramics, traditional and new ceramics, structure of ceramics, atomic interactions a nd types of bonds, phase equilibria in ceramic systems, one component and multi component systems, use of phase diagrams in predicting material behaviour, electrical, magnetic, and optical properties of ceramic materials.

Unit 3: Nanomaterials and Nanotechnology (9hrs)

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

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

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

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

Magnetic materials, ferri and ferro magnetism, metallic magnets, soft, hard & superconducting magnets; Ceramic magnets, low conducting and superconducting magnets; Superconducting materials - metallic and ceramic superconducting materials, theories ofsuperconductivity,

Meissner effect; High temperature superconductors - structure and applications.

Unit 6: Some Special Polymers (9hrs)

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

Unit 7: Composite Materials (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. W.D. Eingery, H.K. Dowen and R.D. Uhlman, *Introduction to Ceramics*, JohnWiley.
2. A.G. Guy, *Essentials of Material Science*, McGrawHill.
3. M.J. Starfield and Shrager, *Introductory Material Science*, McGrawHill.
4. S.K. Hajra Choudhary, *Material Science and Engineering*, Indian Book Dist. Co.,Calcutta.
5. M.W. Barsoum, Fundamentals of Ceramics, McGraw Hill,1997.
6. M. Tinkham, *Introduction to Superconductivity*, McGraw Hill,1975.
7. A.V. Narlikar and S.N.Edbote, *Superconductivity and Superconducting Materials*, South

Asian Publishers, New Delhi,1983.

8. S.V. Subramanyan and E.S. Rajagopal, *High Temperature Superconductors,* Wiley Eastern Ltd.,1988.
9. Azaroff and Brophy, *Electronic Processes in Materials*, McGraw Hill,1985.
10. C.M. Srivastava and C. Srinivasan,Science of Engineering Materials, Wiley Eastern Ltd.,1987.
11. R.J. Young, *Introduction to Polymer Science*, John Wiley andSons.
12. V.R. Gowriker and Others, *Polymer Science*, Wiley EasternLtd.
13. H. Ulrich, *Introduction to Industrial Polymers*, Hansen Publishers,1982.
14. F.R. Jones, *Handbook of Polymer Fibre Composites*, Longman Scientific andTech.
15. K.K. Chowla, *Composite Materials*, Springer-Verlag, NY,1987.

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

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

CHE4E08 – ORGANOMETALLIC CHEMISTRY (ELECTIVE) (4 credits, 72hrs)

COURSE OUTCOME

COURSE: - ORGANOMETALLIC CHEMISTRY (ELECTIVE)
COURSE CODE: CHE4E08
Credits: 4
Total hours: 72
4hrs/week

Sl No	**Course outcomes**	POs/ PSOs	CL	KC
1.	Evaluate the fundamental principles of organotransition-metal chemistry and analyze the influence of metals and ligands on chemical properties.	PSO I	E	F
2.	Evaluate the structure and bonding of organometallic complexes to analyze their stability and reactivity.	PSO I	E	C
3.	Apply modern characterization techniques to identify and characterize organometallic compounds.	PSO II	Ap	C
4.	Analyze fundamental organometallic reaction types and mechanisms and apply them to explain catalytic processes.	PSO I	U	C
5.	Analyze and evaluate the applications of homogeneous organometallic catalysis in the synthesis and production of chemical compounds.	PSO I	An	C
6.	Explain and analyze the mechanisms of organometallic reactions.	PSO III	U	C
7.	Analyze and evaluate the applications of organometallic reactions in chemical synthesis and industrial processes.	PSO V	An	P
8.	Compare and analyze the reactivity of simple organometallic compounds and organometallic polymers.	PSO VI	An	F

Total hours of instruction 72

(**Understand (U) ,Procedural Knowledge (P), Conceptual Knowledge(C),Factual Knowledge(F),Evaluate (E),Analyse (A) ,Apply (Ap))**

UNIT I (9h)

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

UNIT II (9h)

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

UNIT III (9h)

General aspects of synthesis, structure, reactivity and applications of main group organometallic compounds. Metal complexes of NO, H_2, CS, RNC and Phosphines. Metal-carbon multiple bonds - Metal carbenes and carbynes, bridging carbenes and carbynes, N-heterocyclic carbons, multiple bonds to hetero atoms.

UNIT IV (9h)

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

UNIT V (9h)

Applications of organometallic compounds in organic synthesis and homogeneous catalysis, Complex formation and activation of H_2, N_2, O_2, NO by transition metals. Catalytic steps, Oxidative addition, reductive elimination and insertion reactions Hydro zirconation of alkenes and alkynes. Homogeneous catalysis. Hydrogenation, isomerization of alkenes, alkyne, cycloadditions, Zeigler-Natta catalysis, hydro formylation of alkenes, Monsanto acetic acid process and Wacker process. Metal complexes in enantioselective synthesis

UNIT VI (9h)

Organometallic reactions. SN^2 Reactions, Radical Mechanisms, Ionic Mechanisms, σ-Bond Metathesis, Oxidative Coupling and Reductive decoupling, Reactions involving CO, Insertions Involving Alkenes, Other Insertions, α, β, γ and δ Elimination, De insertion 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, Hydro cyanation 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, poly germanes and polys tannanes, 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.

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

M.Sc. CHEMISTRY – SEMESTER III & IV

CHE3L07 & CHE4L10 – INORGANIC CHEMISTRY PRACTICALS– III & IV
(3 Credits)

Sl No	Course outcomes	POs/ PSOs	CL	KC
1.	Perform the quantitative separation and estimation of ions in binary mixtures using volumetric, colorimetric, and gravimetric methods.	PSO V	A	P
2.	Conduct colorimetric estimations of Ni, Cu, Fe, and Mo after separation from interfering ions by solvent extraction and interpret the analytical results.	PSO V	Ap	P
3.	Apply ion-exchange techniques to separate and estimate ions in binary mixtures and determine the hardness of water samples.	PSO VI	Ap	P
4.	Synthesize and characterize inorganic complexes using appropriate experimental and analytical techniques.	PSO VII	C	P

(Apply(Ap),Procedural Knowledge (P),Create (C))

Unit 1: Estimation of ions in mixture

Estimation involving quantitative separation of suitable binary mixtures of ions in solution (Cu^{2+}, Nl^{2+}, Zn^{2+}, Fe^{3+}, Ca^{2+}, Mg^{2+}, Ba^{2+} and Cr2O1^{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*.

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

M.Sc. CHEMISTRY – SEMESTER III & IV

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

Sl No	Course outcomes	POs/ PSOs	CL	KC
1.	Perform and evaluate the quantitative separation and estimation of ions in binary mixtures using volumetric, colorimetric, and gravimetric techniques.	PSO I	Ap	P
2.	Conduct and analyze colorimetric estimations of Ni, Cu, Fe, and Mo following solvent-extraction-based separations.	PSO V	Ap	P
3.	Apply and evaluate ion-exchange methods for the separation and estimation of ions and the determination of water hardness.	PSO VII	C	P

(Apply(Ap),Procedural Knowledge (P),Create (C))

Unit 1: Quantitative Organic Analysis

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

References:

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

Unit 2: Extractions

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

Unit 3: Chromatograhy

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

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

Food colours: Permitted – Amaranth, Erythrosine, Tatrazine, susnet yellow, Fast green, Brilliant Blue, Nonpermitted colours: Auramine, Congo red, Malachite green, Metanil yellow, Orange II, Sudan II, Congo red.

Amino acids (Protein hydrolysates), Sugars, Terpinoids, Alkaloids, Flavonoids, Steroids.

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

Plant growth stimulants: Indole acetic acid.

References:

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

SACRED HEART COLLEGE (AUTONOMOUS), CHALAKUDY

M.Sc. CHEMISTRY – SEMESTER III & IV

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

Sl No	Course outcomes	POs/ PSOs	CL	KC
1.	Apply the principles of chemical kinetics and polarimetry to determine reaction rates and analyze reaction kinetics.	PSO I	Ap	P
2.	Apply adsorption principles to experimentally verify adsorption isotherms and interpret the results.	PSO V	Ap	P
3.	Construct and interpret phase diagrams for different types of systems.	PSO VI	C	P
4.	Apply spectrophotometric techniques for the quantitative analysis of metal ions and evaluate the analytical results.	PSO V	Ap	P
5.	Apply computational chemistry methods to calculate and analyze molecular properties.	PSO II	Ap	P

SECTION A

Unit 1: Chemical Kinetics (4experiments)

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

Unit 2: Adsorption (3 experiments)

1. Verification of Langmuir adsorption isotherm – charcoal-acetic acid system.

Determination of the concentration of a given acetic acid solution using the isotherm

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

Unit 3: Phase Equilibria (2 experiments)

1. (a)Determination of phase diagram of a ternary liquid system (e .g.,chloroform– acetic acid – water – Benzene – acetic acid –water)
   (b) Determination of the composition of a binary liquid mixture (e.g., chloroform-acetic acid, benzene-acetic acid)
2. (a) Determination of mutual miscibility curve of a binary li quid system (e.g., phenol – water) and critical solution temperature(CST).
   (b) Effect of impurities (e.g, NaCl, KCl, succinic acid, salicylic acid) on the CST of water-phenol system
   (c) Effect of a given impurity (e.g., KCl) on the CST of water –phenol system and determination of the concentration of the given solutionof

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

1. Determination of cyroscopic constant of a liquid (water,benzene)
2. Determination of molecular mass of a soute (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 2KI + Hgl 2 .K_2HgI_4 and determination of the concentration of the given KI 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 andK2Cr2O7
3. Investigation of complex formation between Fe (III) and thiocyanate.

References:

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

SECTION B

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

Unit 7: Computational Chemistry Calculations

1. Single point energy calculations of simple molecules like H_2O and NH_3 at the HF/3-21G level of theory.
2. The effect of basis set on the single point energy of H_2O and NH_3 using the Hartree-Fock method (3-21G, 6-31G, 6-31+G, 6-31+G* basis sets can be used).
3. Geometry optimization of molecules like H_2O, NH_3, HCHO & C_2H_4 at the HF/6-31G level of theory.
4. Computation of dipole and quadrupole moments of HCHO& C_2H_4 at the HF/6-31G level of theory.
5. Effect of basis set on the computation of H-O-H bond angle in H_2Ousing the Hartree -Fock method (3-21G, 6-31G, 6-31+G, 6-31+G* basis sets can be used).
6. Computation of the energy of HOMO and LUMO of formaldehyde and 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 H_2O_2at 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 likeH_2O, NH_3 and CO_2at the HF/6-31+G* level of theory.
11. Determination of hydrogen bond strength of H_2O dimer and H_2O trimer at the HF/6-31+G* level of theory.
12. 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