ST. THOMAS' COLLEGE (AUTONOMOUS)
THRISSUR, KERALA – 680001

Affiliated to University of Calicut
Nationally reaccredited with 'A' Grade

CURRICULUM AND SYLLABUS
FOR
POSTGRADUATE PROGRAMME IN CHEMISTRY

UNDER CHOICE BASED CREDIT AND SEMESTER SYSTEM
(w.e.f. 2020 Admission onwards)

ST. THOMAS COLLEGE (AUTONOMOUS), THRISSUR

OUTCOME BASED EDUCATION

POST GRADUATE PROGRAM OUTCOMES

At the end of Post Graduate Program at St. Thomas College (Autonomous), a student would have:

PO1:	Attained profound **Expertise in Discipline**.
PO2:	Acquired **Ability to function in multidisciplinary Domains**.
PO3:	Attained ability to exercise **Research Intelligence** in investigations and Innovations.
PO4:	Learnt Ethical Principles and be committed to **Professional Ethics**.
PO5:	Incorporated **Self-directed and Life-long Learning**.
PO6:	Obtained Ability to maneuver in diverse contexts with **Global Perspective**.
PO7:	Attained **Maturity to respond to one’s calling**.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

M.Sc. CHEMISTRY (CBCSS PATTERN)

Regulations and Syllabus with effect from 2020 admission

The Board of Studies in Chemistry at its meeting held on 15-05-2019 considered the revision of M.Sc. Chemistry syllabus under Credit Semester System (CBCSS) and resolved to implement the revised syllabus from 2020 admission onwards. The revised programme pattern; syllabus, distribution of credits and scheme of evaluation, etc. approved by the Board of studies in Chemistry at its meeting held on **12-12-2019** are given below:

The pattern of the Programme

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

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

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

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

Theory Courses

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

Practical Courses

In each semester, there will be three core practical courses. However, the practical examinations will be conducted only at the end of the second and fourth semesters. At the end of the 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 the fourth semester. **Each practical examination will be of six-hour duration with 3 credits. Three hours per week in the fourth semester are allotted for conducting individual project work by the students under the guidance of a faculty and it can be treated as practical hours while calculating the workload of teachers.**

Project and Viva-Voce

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

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

(4) Evaluation and Grading should be done by the direct grading system. All grading during the evaluation of courses and the semester is done on a 6-point scale (A+, A, B, C, D, E). Grading in the 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 a 10-point scale as detailed below.

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

Pass in a course: P grade and above (GPA 2.00 and above). Pass in all courses in a semester is compulsory to calculate the SGPA.GPA, SGPA, and CGPA will be between 0 to 5 and in two decimal points. An overall letter grade (Cumulative Grade) for the whole programme shall be awarded to the student based on the value of CGPA using a 10-point scale given below.

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

(5) Weightage of Internal and External valuation:

The evaluation scheme for each course shall contain two parts

(a) Internal evaluation

(b) External evaluation.

Its weightages are as follows:

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

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

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

Theory: 5 weightages

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

(b) Assignments and Exercises- weightage =1

i. Seminars/Viva Voce- weightage =1

ii. Attendance –weightage =1

Practical: 10 weightages

a) Attendance – weightage =2

b) Lab. skill/quality of their results- weightage =2

c) Model practical test-weightage = 2 (Best one, out of two model exams is considered)

d) Record-weightage =2

e) Viva Voce- weightage =2

Project: 10 weightages

a) Literature survey and data collection-weightage =2

b) Interpretation of data & Preparation of Project report – weightage =2

c) Research attitude - weightage =2

d) Viva Voce- weightage =4

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

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

Attendance: Above 90 %: A+, 85 – 89.99 %: A, 80 – 84.99 %: B,

75 -79.99 %: C, 70– 74.99%: D, < 70%: E

(7) External evaluation:

a) **Theory**: In all semesters the theory courses have 30 weightage each. The pattern of Question Papers for theory courses is as follows

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

Total weightage in question paper 30

b) **Practicals**: At the end of II and IV semesters, there will be three practical examinations. Each examination has 30 weightage and 3credits

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 of the programme.

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

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

Evaluation is based on:

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

Total weightage 30 and credit for the project is 4.

(8) Directions for question 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 Modules 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 University PG regulations 2019)

Audit courses:

Ability Enhancement Course (AEC):

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

AEC is a 4 credit course and should be conducted during the first semester of the programme. The 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 an overall pass in the programme.

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

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

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

Professional Competency Course (PCC):

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

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

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

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

a) Development of skills on using softwares like Gaussian, Gamessetc which is useful in molecular modeling, drug designing etc.
b) Development of skills on using softwares like Chemdraw, Chemwindow, ISIS draw, etc which is useful in drawing purposes, structural predictions,etc.
c) Training on computational chemistry
d) Case study and analysis on any relevant issues in the nearby society(for example water analysis, soil analysis, acid/alkali content analysis, sugar content analysis, etc)
e) Any commModuley linking programme relevant to the area of study(For example Training for society on soap/perfume making, waste disposal, plastic recycling, etc)

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

Research Awareness: SECOND SEMESTER M Sc CHEMISTRY

Acquiring the basic knowledge on research is inevitable during the course of postgraduate programme. Awareness on the different essential steps of research and current scenario of research in chemical science area is to be imparted during the M.Sc chemistry programme. Based on this concept, following components are introduced in the syllabus and curriculum to promote research culture in the stakeholders especially PG students.

During second semester each student has to utilize research journals available in the library as well as in the websites and submit an assignment on any research article/reviews published in the journals. A committee comprised of 1) teacher in charge of the student on research project, 2) Teacher in charge of the batch & 3) Head of the department has to assess the assignment and grade it.

Each student has to present a seminar on the above assignment in consultation with the teacher in charge of the research project and the above committee has to evaluate the same and grade it.

Evaluation and grading may be done as in the case of assignment and seminar, concerned with the theory courses

M.Sc Project work, minimum of two months duration, must be carried out by each student under the supervision of a teacher in charge of research, in a reputed research institution outside the college, as possible. The project work should be carried out during the month of April and May, immediately after the second semester examinations.

Analytical and Local issue awareness: FOURTH SEMESTER M.Sc CHEMISTRY

Each student has to submit an assignment on any local issues related to chemical science area during the fourth semester of the M.Sc chemistry programme. Or an assignment on the use of any particular advanced analytical instruments which have wide applications in research as well as in analyzing and solving a local issue. A committee comprised of 1) teacher in charge of the student on research project, 2) Teacher in charge of the batch and 3) Head of the department has to assess the assignment and grade it.

Each student has to present a seminar on the above assignment in consultation with the teacher in charge of the research project and the above committee has to evaluate the same and grade it. Evaluation and grading may be done as in the case of assignment and seminar, concerned with the theory courses.

	PROGRAMME SPECIFIC OUTCOMES (PSO) M.Sc CHEMISTRY PROGRAMME
PSO1	Understand the concepts of quantum mechanics, thermodynamics, electrochemistry and petrochemicals
PSO2	Understand the concepts of computational chemistry, group theory, coordination chemistry and molecular spectroscopy with the emphasis on problem solving.
PSO3	Understand advanced topics in inorganic, physical, organic and theoretical chemistry.
PSO4	Understand the advanced concepts in inorganic, physical and organic and analyze these concepts in chemical experiments.

TABLE 1

Courses offered for M.Sc. Chemistry Programme under CBCSS Patten

(2020 onwards)

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

III	CHE3L07	Inorganic chemistry practical III	4	
	CHE3L08	Organic chemistry practical III	4	
	CHE3L09	Physical chemistry practical III	4	
	CHE3E01	Synthetic organic chemistry(Elective)	3	4
	CHE3E02	Computational chemistry(Elective)	3	4
	CHE3E03	Green and Nanochemistry(Elective)	3	4
		Total Credits: 16	**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 & Polymer Chemistry (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: 27	**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**

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

CHE1C01 - QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY (4 Credits, 72 h)

CO1	Understand the broad frame work of quantum mechanical theory
CO2	Understand the limitations of Schrodinger equations
CO3	Understand the approximation methods for multi electron atoms
CO4	Understand the approximation methods for molecules
CO5	Understand the origin of atomic orbitals
CO6	Analyze simple microscopic systems by solving Schrodinger equation
CO7	Apply the approximation methods to multi electron atoms
CO8	Evaluate molecular parameters using Gaussian programme

Module 1: Introduction to Quantum Mechanics (9h)

Black body radiation and Planck's interpretation. 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 functions; Operator postulate, operator algebra, linear and nonlinear operators, Non-commuting operators and the Heisenberg's Uncertainty principle, Conserved properties and the Hamiltonian operator. 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, and time- independent Schrödinger equation. Stationary states and bound states.

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

Free particle in one-dimension; Particle in a one-dimensional box with infinite potential walls, important features of the problem; Particle in a rectangular well (no derivation); Quantum mechanical tunneling of a free particle against a 1D potential barrier of finite height and width. Particle in a three dimensional box, Separation of variables, degeneracy.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.

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

Co-ordinate systems: - Cartesian, and spherical polar coordinates and their relationships. Planar rigid rotor (or particle on a ring), the Phi-equation, solution 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 ((Lx, Ly, Lz), commutation relations between these operators, space quantization.

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

Potential energy of hydrogen-like systems, the wave equation in spherical polar coordinates, separation of variables, the R, Theta and Phi equations and their solutions, Laguerre and associated Laguerre polynomials, wave functions and energies of hydrogen-like atoms, orbitals, radial functions and radial distribution functions and their plots, angular functions (spherical harmonics) and their plots. Discovery of spin: Stern-Gerlach experiment and interpretation of the result (qualitative treatment), spin orbitals, construction of spin orbitals from orbitals and spinfunctions.

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

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

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

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

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

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

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

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

Reference (for Modules 1 to 6)

1. F.L. Pilar, Elementary Quantum Chemistry, McGraw-Hill, 1968.
2. I.N. Levine, Quantum Chemistry, 6th Edition, Pearson Education Inc.,
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, Vivabooks, 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 many derivations).
11. R.L. Flurry, Jr., Quantum Chemistry, Prentice Hall, 1983.
12. R.K. Prasad, Quantum Chemistry, 3rd Edition, New Age International, 2006.
13. M.S. Pathania, Quantum Chemistry, and Spectroscopy (Problems & Solutions), Vishal Publications, 1984.
14. C.N. Datta, Lectures on Chemical Bonding and Quantum Chemistry, Prism Books Pvt. Ltd. 1998.
15. Jack Simons, An Introduction to Theoretical Chemistry, Cambridge University Press, 2003.

Reference (for Modules 7 & 8)

1. C. J. Cramer, Essentials of computational Chemistry: Theories and models, John Wiley & Sons 2002.
2. Frank Jensen, Introduction to Computational Chemistry, John Wiley & Sons LTD1999.
3. J. Foresman & Aelieen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
4. David Young, Computational Chemistry- A Practical Guide for Applying Techniques to Real- World Problems", Wiley -Interscience, 2001.
5. Errol G. Lewars, Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics, 2 ndedn., Springer 2011.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER I

CHE1C02 - - ELEMENTARY INORGANIC CHEMISTRY (4 Credits, 54h)

CO1	Compare bonding in P-N, P-S and S-N compounds.
CO2	Rationalize the acidic/basic behavior of substances in different solvents.
CO3	Apply Wade's rule to predict structure of Boron clusters.
CO4	Apply Styx numbers to predict polyhedral structure.
CO5	Predict theoretical magnetic moment of lanthanides.
CO6	Predict the products of a nuclear fission reaction.
CO7	Predict disproportionation of oxides based on Latimer diagram.
CO8	Evaluate suitable characterization techniques for a given nanomaterial.

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

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

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

Chemical periodicity-First and Second row anomalies-The diagonal relationship-Periodic anomalies of the nonmetals and post-transition metals.
Allotropes of C, S, P. As, Sb, Bi, O, and Se. Electron-deficient compounds-Boron hydrides-preparation, reactions, structure, and bonding. Styx numbers-closo, nido, arachno polyhedral structures. Boron cluster compounds-Wade's rule. Polyhedral borane anion-carboranes, metallaboranes and metallacarboranes. Borazines and borides.
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Module 3: Chemistry of Main Group Elements-II (9h)

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

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

Heteropoly and isopoly anions of W, Mo, V: Strandberg, Keggin, decavanadate and Anderson (only). 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

Module 5: Nuclear and Radiation Chemistry (9h)

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

Module 6: Chemistry of Nanomaterials (9h)

History of nanomaterials - Classification. Size - dependence of properties. Synthesis of nanostructures: bottom-up-approach, top-down approach, self-assembly, lithography, molecular synthesis, template-assisted synthesis.Methods of characterization: Electron microscopies-SEM, TEM. Scanning probe microscopies- STM, AFM. X-ray photoelectron spectroscopy (XPS), Dynamic light scattering (DLS), and X-ray diffraction (XRD). Applications: Nanoelectronics, nanosensors, nanocatalysts, nanofiltration, diagnostic and therapeutic applications, and targeted drug delivery. Introduction to graphenes and fullerenes.

Reference (for Modules 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.
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References (for Module 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, RSC Publishing, 2008.
3. T.Pradeep, The essentials of Nanotechnology, Tata McGraw-Hill, New Delhi, 2007.
4. K.J.Klabunde (Ed.), Nanoscale Materials in Chemistry, John Wiley& Sons, 2001.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

CHE1C03 - STRUCTURE, AND REACTIVITY OF ORGANIC COMPOUNDS
(4 Credits, 54h)

CO1	Understand structure, bonding and stability of organic molecules.
CO2	Understand the theories of reactivity based on structure.
CO3	Understand the methods of conformational analysis
CO4	Understand the basic models for applications of stereochemistry.
CO5	Apply the methods of conformational analysis in organic reactions.
CO6	Predict the stereochemistry of products in asymmetric synthesis.

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

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

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

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

Module 2: Structure and Reactivity (9h)

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

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

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

Module 3: Conformational Analysis – I (9h)

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

Interconversion of axial and equatorial bonds in chair conformation of cylohexane– distance between the various H atoms and C atoms in chair and boat conformations. Monosubstituted cyclohexane–methyl and t-butyl cyclohexanes–flexible and rigid systems. Confirmation of substituted cyclohexanone, 2-bromocyclohexanone, dibromocyclohexanone, (cis & trans), 2-bromo-4, 4-dimethyl cyclohexanone. Optical activity in cis-trans conformational isomers of 1, 2-, 1, 3- and 1,4-dimethylcyclohexanes. Anchoring group and conformationaly biased molecules. Conformations of 1, 4 -cis and-trans disubstituted cyclohexanes in which one of the substituents is 1-butyl and their importance in assessing the reactivity of an axial or equatorial substituent.

Module 4: Conformational Analysis – II (9 h)

Effect of conformation on the course and rate of reactions in (a) debromination of dl and meso 2, 3-dibromobutane or stilbene dibromide using KI. (b) semipinacolic deamination of erythro and threo 1,2-diphenyl-1-(p-chlorophenyl)-2-aminoethanol.
(c) dehydrohalogenation of stilbene dihalide (dl and meso) and erythro and threo-bromo-1,2-diphenyl propane.
Effect of conformation on the course and rate of reactions in cyclohexane systems illustrated by (a) 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 as equatorial carboxyl groups and hydrolysis of their esters. (g) Hydrolysis of axial and equatorial tosylates. (h) Oxidation of axial and equatorial hydroxyl group to ketones by chromic acid.

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

Module 5: Stereochemistry (9h)

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

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

Optical isomerism in biphenyls, allenes, spirans and nitrogen and sulphur compounds, conditions for optical activity, R and S notations. Restricted rotation in biphenyls – Molecular overcrowding. Chirality due to the folding of helical structures.

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

Module 6: Asymmetric Synthesis (9 h)

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

Classification of Asymmetric reactions into (1) Substrate controlled (2) Chiral auxiliary controlled (3) Chiral reagent controlled and (4) Chiral catalyst controlled. Substrate controlled asymmetric synthesis: Nucleophillic addition to chiral carbonyl compounds. 1, 2-asymmetric induction, Cram's rule and Felkin- Anhmodel. 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.Chiral reagent controlled asymmetric synthesis: Asymmetric reduction using BINAL– H. Asymmetric hydroboration using IPC_2BH and $IPCBH_2$. Reduction with CBH reagent. Stereochemistry of Sharpless asymmetric epoxidation and dihydroxylation. Asymmetric aldol reaction: Diastereoselective aldol reaction and its explanation by Zimmermann-*Traxler* model. Auxillary controlled aldol reaction. Double diastereoselection-matched and mismatched aldol

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.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

CHE1C04 – THERMODYNAMICS, KINETICS AND CATALYSIS (4 Credits, 54h)

CO1	Understand the laws of thermodynamics
CO2	Understand the importance of catalysis in industrial processes
CO3	Analyze the important theories of chemical kinetics
CO4	Apply the thermodynamical principles to irreversible processes
CO5	Apply the principles of chemical kinetics to complex reaction mechanisms

Module 1: Thermodynamics (9h)

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

Module 2: Thermodynamics of Irreversible Processes (9 h)

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

Module 3: Chemical Kinetics (9 h)

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

Module 4: Molecular Reaction Dynamics (9 h)

Reactive encounters: Collision theory, diffusion-controlled reactions, the material balance equation, Activated Complex theory – the Eyring equation, thermodynamic aspects of ACT; Comparison of collision and activated complex theories; The dynamics of molecular collisions. 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.

Module 5: Surface Chemistry (9 h)

Structure and chemical nature of surfaces, Adsorption at surfaces - Adsorption isotherms, Langmuir's unimolecular theory of adsorption, competitive adsorption, dissociative adsorption, BET equation, derivation, V_{mono} calculation. 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.

Module 6: Catalysis (9h)

Features of homogeneous catalysis–Enzyme catalysis - Michaelis-Menten Mechanism.Features of heterogeneous catalysis -Langmuir-Hinshelwood mechanism and Eley-Rideal mechanism – illustration using the reaction $2CO + O_2$---› $2CO_2$. Auto catalysis - oscillating reactions – mechanisms of oscillating reactions (Lotko -Volterra, brusselator, and oregonator). Applied Catalysis: Haber-Bosch process, Fischer-Tropsch process and Three-way automotive catalyst. Catalytic poisons and promotors

References

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, 2nd edition, 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, Prentice Hall of India.
9. M.K. Adam, The Physics and Chemistry of surfaces , Dover Publications

10. S. Glasstone, Thermodynamics for chemists, East-West 1973.
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 of India
14. A. W. Adamson and A. P. Gast, Physical Chemistry of Surfaces, 6th 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, 2ndEdn. 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.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

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

CO1	Understand the concept of symmetry operations, point group.
CO2	Ability to generate a set of representations.
CO3	Construction of character table using group theory.
CO4	Analyse the spectroscopic properties of molecules using theory.
CO5	Application of group theory principles and chemical bonding.
CO6	Applications of MO & VB theories and Huckel M.O. calculations.

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

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

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

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

Module 3: Applications of Group Theory to Molecular Spectroscopy (9h)
Molecular vibrations - symmetry species of normal modes of vibration, construction of Γ_{cart}, normal coordinates and drawings of normal modes (e.g., H_2O and NH_3), selection rules for IR and Raman activities based on symmetry arguments, determination of IR active and Raman active modes of molecules (e.g., H_2O, NH_3, CH_4 , SF_6), complementary character of IR and Raman spectra.
Spectral transition probabilities - direct product of irreducible representations and its use in identifying vanishing and non–vanishing integrals, transition moment integral and spectral transition probabilities.
Electronic Spectra – electronic transitions and selection rules, Laporte selection rule for centro symmetric molecules.

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

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

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

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

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

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

References (for Modules 1 to 4)

1. F.A. Cotton, Chemical applications of Group Theory, 3rd Edition, 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.

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6. Mark Ladd, Symmetry & Group Theory in Chemistry, Horwood, 1998.
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 Academic Publishers, 2004.
9. K. Veera Reddy, Symmetry & Spectroscopy of Molecules 2^{nd} Edn., New Age International 2009.
10. A.W. Joshi, Elements of Group Theory for Physicists, New Age International Publishers, 1997.

References (for Modules 5 &6)

1. F.L. Pilar, Elementary Quantum Chemistry, McGraw-Hill, 1968.
2. I.N. Levine, Quantum Chemistry, 6th Edition, Pearson Education Inc.,
3. P.W. Atkins and R.S. Friedman, Molecular Quantum Mechanics, 4^{th} Edition, Oxford University Press, 2005.
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ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

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

CO1	Compare the stability of complexes.
CO2	Compare the splitting of d-orbitals in different fields.
CO3	Derive d^n configurations.
CO4	Apply 18 electron rule in metal carbonyls.
CO5	Apply redox properties of $[Ru(bipy)_3]^{2+}$ to understand water photolysis.
CO6	Predict the nature of substitution based on trans effect.

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

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

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

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

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

Module 4: Characterization of Coordination Complexes (9h)
Infrared spectra of metal complexes. Group frequency concept. Changes in ligand

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

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

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

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

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

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

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

References:

1. N.N.Greenwood and A.Earnshaw, Chemistry of Elements, 2/e, Butterworth-Heinemann, 2005.
2 J.E. Huheey, E.A. Keiter, R.L. Keiter and O.K. Medhi, Inorganic Chemistry, principles of structure and reactivity, Pearson Education, 2006.
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ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

CHE2C07 - REACTION MECHANISM IN ORGANIC CHEMISTRY (3 Credits, 54h)

CO1	Understand common substitution and elimination reactions.
CO2	Interpret structure and synthesis of various natural products.
CO3	Analyse the role of intermediates in common reactions.
CO4	Analyse the mechanistic aspects of various name reactions.
CO5	Apply the principles of pericyclic reactions.
CO6	Apply the photochemical reactions in various organic molecules.

Module 1: Aliphatic and Aromatic Substitutions (9 h)

Nucleophilic Aliphatic Substitution: Mechanism and Stereochemistry of S_N2 and S_N1 reactions. Ion-pair mechanism. The effect of substrate structure, reaction medium, nature of leaving group and nucleophile on S_N2 and S_N1 reactions. S_Ni and neighboring group mechanism. SET mechanism. Allylic and benzylic substitutions. Ambident nucleophiles and substrates regioselectivity.
Electrophilic Aliphatic Substitution: Mechanism and stereochemistry of S_E1, S_E2 (front), S_E2 (back) and S_Ei reactions. The effect of substrate structure, leaving group and reaction medium on S_E1 and S_E2 reactions.
Electrophilic Aromatic Substitution: Arenium ion mechanism, substituent effect on reactivity in mono and disubstituted benzene rings, *ortho/para* ratio, *Ipso* substitution. Relationship between reactivity and selectivity. Nucleophilic Aromatic substitution: Addition- elimination (S_NAr) mechanism, elimination-addition (benzyne) mechanism, *cine* substitution, S_N1 and $S_{RN}1$ mechanism. The effect of substrate structure, nucleophile and leaving group on aromatic nucleophilic substitution.

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

(i) Addition and Elimination Reactions (6h)

Mechanistic and stereochemical aspects of addition to C=C involving electrophiles, nucleophiles and free radicals. Effect of substituents on the rate of addition, orientation of addition, addition to conjugated systems and cyclopropane rings, Michael reaction.
Mechanistic and stereochemical aspects of E1, E1cB and E2 eliminations. The effect of substrate structure, base, leaving group and reaction medium on elimination reactions. Saytzev *vs* Hofmann elimination, α- elimination, pyrolytic *syn* elimination (E*i*) and conjugate eliminations. Competition between substitution and elimination reactions, basicity *vs* nucleophilicity. Extrusion reactions- extrusion of N_2, CO and CO_2.

(ii) Reactive Intermediates (3hrs)

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

Module 3: Chemistry of Carbonyl Compounds (9h)

(i) Reactions of Carbon-heteromultiple Bonds (7h)
Reactivity of carbonyl compounds toward addition, mechanistic aspects of hydration, addition of alcohols, and condensation with nitrogen nucleophiles to aldehydes and ketones. Addition of organometallic reagents- Grignard reagents- organozinc, organocopper and organolithium reagents- to carbonyl compounds. Aldol, Perkin, Claison, Dieckmann, Stobbe, and benzoin condensation. Darzen's, Knoevenagel, Reformatsky, Wittig, Cannizaro, Mannich, and Prins reactions. MPV reduction and Oppenauer oxidation.
Addition to carbon-nitrogen multiple bonds: Ritter reaction and Thorpe condensation. Hydrolysis, alcoholysis, and reduction of nitriles.
(ii) Esterification and Ester Hydrolysis (2h): Mechanisms of ester hydrolysis and esterification, Acyl-oxygen and alkyl oxygen cleavage.

Module 4: Pericyclic Reactions (9 h)
Phase and symmetry of molecular orbitals, FMOs of ethylene, 1, 3- butadiene, 1, 3, 5- hexatriene, allyl, and 1, 3-pentadienyl systems. Pericyclic reactions: electrocyclic, cycloaddition, sigmatropic, chelotropic and group transfer reactions. Theoretical models of pericyclic reactions: TS aromaticity method (Dewar- Zimmerman approach), FMO method and Correlation diagram method (Woodward- Hoffmann approach). Woodward- Hoffmann selection rules for electrocyclic, cycloaddition and sigmatropic reactions. Stereochemistry of Diels- Alder reactions and regioselectivity. Cope and Claison rearrangements. Stereochemistry of cope rearrangement and valence tautomerism. 1, 3- dipolar cycloaddition reactions and *ene* reactions.

Module 5: Photochemistry of Organic Compounds (9 h)
Photochemical excitation of molecules, spin multiplicity, Jablonski diagram, photosensitization, and quenching. Photochemistry of carbonyl compounds: Norrish type- I cleavage of acyclic, cyclic and β, γ- unsaturated carbonyl compounds, β-cleavage, γ- hydrogen abstraction: Norrish type- II cleavage, photo reduction, photoenolization. Photocyclo- addition of ketones with unsaturated compounds: Paterno- Büchi reaction, photodimerization of α, β- unsaturated ketones, Photo rearrangemets: Photo –Fries, di- π- methane, lumi ketone, oxa di- π- methane rearrangements. Barton and Hoffmann- Loeffler- Freytag reactions. Photo isomerization and dimerization of alkenes, photo isomerization of benzene and substituted benzenes, photooxygenation.

Module 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, Academic Press, 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.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

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

CO1	Understand the important principles of statistical thermodynamics
CO2	Understand the theory of over-voltage
CO3	Understand the electronic structure of crystalline solids
CO4	Apply the electrochemical principles to batteries
CO5	Apply the principles of statistical thermodynamics to the physical properties of system

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

Anomalous behavior of strong electrolytes, Theory of strong electrolytes, Ionic atmosphere, The Debye-Hückel equation, Deviation from Debye-Huckel equation, Activity and activity coefficient of electrolytes, Ionic strength, Limiting and extended forms of the Debye- Hückel equation, Applications of the Debye-Hückel equation for the determination of thermodynamic equilibrium constants and to calculate the effect of ionic strength on ion reaction rates in solution.

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

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

Module 2: Dynamic Electrochemistry (9h)

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

Module 3: Solid State – I (9h)

Crystal symmetry: Symmetry elements and symmetry operations, mathematical proof for the non-existence of 5-fold axis of symmetry, crystal systems, Bravais lattices and crystal classes, Crystallographic point groups – Schönflies & Hermann–Mauguin notations, Stereographic projections of the crystallographic point groups (C_n, D_n, O, T, C_{nh}, C_{nv}), translational symmetry elements & symmetry operations - screw axes and glide planes, introduction to space groups. Reciprocal Lattice and Reciprocal lattice vector. Ewald sphere construction and condition for diffraction. Geometric structure factor.

Module 4: Solid State – II (9h)

Electronic structure of solids: Bloch Function, **k** vector, Brillouin zone, Band width, Band structure, Effective mass, Dispersion of band formed from s orbitals (1D case), Dispersion of band formed from p orbitals (1D case), Example of band structure of Eclipsed Stack of Pt(II) Square Planar Complex, Fermi level and Density of States of $\{[PtH4]^{2-}\}\infty$. Special **k** points in the for the Brillouin zone of primitive cubic, fcc, and bcc. Bloch's Theorem, Free-Electron Dispersion, Electrons in a Periodic Potential. Band–Band Transitions: Energy Gap, Direct Transitions, Indirect Transitions.

Module 5: Statistical Thermodynamics- I (9h)

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

Module 6: Statistical Thermodynamics- II (9h)

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

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

References

For Modules 1-4

1. D. R. Crow, Principles and Applications of Electrochemistry, Chapman and Hall London, 1979.
2. J.O.M. Bockrisand A.K.N. Reddy, Modern Electrochemistry, Vol. I and II, Kluwer Academic / Plenum Publishers, 2000.
3. Carl. H. Hamann, A. Hamnett, W.Vielstich, Electrochemistry 2nd edn. , Wiley-VCH, 2007.
4. Philip H Reiger, Electrochemistry 2nd edn. , Chapman & Hall, 1994.
5. Praveen Tyagi, Electrochemistry, Discovery Publishing House, 2006.
6. D.A. McInnes, The Principles of Electrochemistry, Dover publications, 1961.
7. L.V. Azaroff, Introduction to Solids, McGraw Hill, NY, 1 960.
8. A.R. West, Basic Solid State Chemistry 2nd edn. , John Wiley & Sons, 1999.

3. A.R. West, Solid State Chemistry & its Applications, John Wiley & Sons, 2003 (Reprint 2007).
4. Charles Kittel, Introduction to Solid State Physics, 7th edn, John Wiley & Sons, 2004 (Reprint 2009).
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., Springer 2004.
9. N.B. Hanna, Solid state Chemistry, Prentice Hall
10. Roald Hoffmann, How Chemistry and Physics Meet in the Solid State, Angew. Chem. Int. Ed. 1987, 26, 846.
11. The Physics of Semiconductors: An Introduction Including Devices and Nanophysics, Marius Grundmann, Springer, Berlin, 2006.

For Modules 5 & 6

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

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR
M.Sc. CHEMISTRY – SEMESTER I&II

CHE1L01 & CHE2L04 – INORGANIC CHEMISTRY PRACTICALS– I & II (3 Credits)

CO1	Enable students to identify rare elements in a sample.
CO2	Enable the students to develop analytical skills.
CO3	Gain expertise in preparation of standard solutions.
CO4	Acquire skills in quantitative calorimetric analysis.
CO5	Apply acquired skills to analyse quality of potable water and food samples.
CO6	Apply the basic concept of inter group separation to identify cations in a given mixture.

MODULE 1: Inorganic Cation Mixture Analysis

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

MODULE 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+})

MODULE 3: Colorimetric Analysis

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

MODULE 4: Experiments with social relevance

1. Determination of water quality parameters.
2. Qualitative analysis of common adulterants in food.

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 MacmillanCompany, 1969.
4. R.A. Day (Jr.) and A.L. Underwood, Quantitative Analysis, 6th Edition, Prentice Hall of India, 1993.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

M.Sc. CHEMISTRY – SEMESTER I &II

CHE1L02 & CHE2L05 – ORGANIC CHEMISTRY PRACTICALS– I & II (3 Credits)

CO1	Practice various purification techniques.
CO2	Prepare organic compounds by multistage methods.
CO3	Enable functional group analysis.
CO4	Determine the physical constants of organic compounds.
CO5	Analyse organic binary mixture.
CO6	Apply organic qualitative analysis by microscale techniques.

Module 1: Laboratory Techniques

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

Module 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.

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

References

1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, 5/e, Pearson,1989.
2. Shriner, FusonandCartin, Systematic Identification of Organic Compounds, 1964.
3. Fieser, Experiments in Organic Chemistry,1957.
4. Dey, Sitaraman and Govindachari, A Laboratory Manual of Organic Chemistry, 3rdEdition,1957.
5. P.R. Singh, D.C. Gupta, and K.S. Bajpal, Experimental Organic Chemistry, Vol. I and II,1980.
6. Vishnoi, Practical 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 and Co., 2010.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

M.Sc. CHEMISTRY – SEMESTER I & II

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

CO1	Determine the molarheat of solution of a substance
CO2	Determine phase diagram of a simple eutectic system
CO3	Determine phase diagram of a binary solid system forming a compound
CO4	Determine molar refractions of pure liquids
CO5	Determine strength of acids/bases using conductometric/ potentiometric titrations
CO6	Apply principles of viscosity to determine molecular weight of a polymer
CO7	Apply refractometry to determine of the composition of liquid mixtures

SECTION A

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

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

Module 2: Phase Equilibria (minimum 3 experiments)

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

Module 3: Viscosity (minimum 2 experiments)

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

Module 4: Distribution Law (minimum 3 experiments)

1. Determination of distribution coefficient of I_2 between CCl_4 andH_2O.
2. Determination of equilibrium constant of $KI + I_2 = KI_3$
3. Determination of concentration of KI solution.

SECTION B

Module 5: Refractometry (minimum 3 experiments)

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

Module 6: Conductivity (minimum 4 experiments)

1. Determination of equivalent conductance of a weak electrolyte (e.g., acetic acid), verification of Ostwald's dilution law and calculation of dissociation constant.
2. Determination of solubility product of a sparingly soluble salt (e.g. AgCl, $BaSO_4$)
3. Conductometric titrations

(a) HCl vs NaOH

(b) (HCl + CH_3COOH) vs NaOH

4. Determination of the degree of hydrolysis of aniline hydrochloride

Module 7: Potentiometry (minimum 3 experiments)

1. Potentiometric titration: HCl vs NaOH, CH_3COOH vs NaOH
2. Redox titration: KI vs $KMnO_4$, $FeSO_4$ vs$K_2Cr_2O_7$
3. Determination of dissociation constant of acetic acid by potentiometric titration
4. Determination of pH of weak acid using Potentiometry
5. Determination of pH of acids and bases using pH meter

References

1. A. Finlay, Practical Physical Chemistry, Longman's Green&Co.
2. J.B. Firth, Practical Physical Chemistry, Read Books(Reprint2008).
3. A.M. James, Practical Physical Chemistry, Longman, 1974.
4. F.Daniel,J.W.Williams,P.Bender,R.A.Alberty,C.D.CornwellandJ.E.Harriman, Experimental Physical Chemistry, McGraw Hill, 1970.
5. W.G. Palmer, Experimental Physical Chemistry, 2nd Edition, Cambridge University Press,1962.
6. D.P. Shoemaker and C.W. Garland, Experimental Physical Chemistry,McGraw-Hill.
7. J. B. Yadav, Advanced Practical Physical Chemistry, GoelPublications, 1989.
8. B. Viswanathan & R.S. Raghavan, Practical Physical Chemistry, Viva Books, 2009.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

CHE3C09 - MOLECULAR SPECTROSCOPY (4 Credits, 72h)

CO1	Understand the fundamentals of spectroscopy.
CO2	Understand theory and applications of NMR techniques.
CO3	Familiarize the principles and applications of Mossbauer Spectroscopy.
CO4	Correlate mass spectral data to the structure of organic compounds.
CO5	Apply Raman, IR and electronic spectra in structural analysis.
CO6	Apply basic principle of microwave spectroscopy.
CO7	Analyse various spectral data.
CO8	Elucidate the structure using spectral data.

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

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

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

Vibrational spectroscopy: Normal modes of vibration of a molecule, vibrational spectra of diatomic molecules, anharmonicity, Morse potential, fundamentals, overtones, hot bands, combination bands, difference bands, vibrational spectra of polyatomic molecules, Vibration- rotation spectra of diatomic and polyatomic molecules, spectral branches -P, Q & Rbranches.
*Raman spectroscopy***:** Classical and Quantum theory of Raman Effect Pure rotational & pure vibrational Raman spectra, vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Introduction to Resonance Raman spectroscopy (basics only).
Electronic Spectroscopy: Characteristics of electronic transitions – Vibrational coarse structure, intensity of electronic transitions, Franck - Condon principle, types of electronic transitions, Dissociation and pre-dissociation, Ground and excited electronic states of diatomic molecules, Electronic spectra of polyatomic molecules, Electronic spectra of conjugated molecules.

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

NMR: Quantum mechanical description of Energy levels-Population of energy-Transition probabilities using ladder operators, Nuclear shielding, Chemical shift, Spin-Spin coupling and splitting of NMR signals, Quantum mechanical Description- AX and AB NMR pattern.

Effect of Relative magnitudes of J (Spin-Spin coupling) and Chemical Shift on the spectrum of AB type molecule. Karplus relationship. Nuclear Overhauser Effect- FT NMR- Pulse sequence for T1 and T2 (Relaxation) measurements.

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

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

Mossbauer Spectroscopy: The Mossbauer Effect, Doppler effect, Doppler broadening, hyperfine interactions, isomer shift, electric quadruple and magnetic hyperfineinteractions. Mossbauer spectra of Iron complexes.

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

UV-Visible spectroscopy: Factors affecting the position and intensity of electronic absorption bands – conjugation, solvent polarity and steric parameters. Empirical rules for calculating $\lambda_{max}$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 andaxial haloketone rule for the determination of conformation and configuration of 3-methyl cyclohexanone and *cis*- and *trans*-decalones. CD curves.
Infrared Spectroscopy: Functional group and finger print regions, Factors affecting vibrational frequency: Conjugation, Vibrational coupling, electronic, steric, ring strain and hydrogen bonding. Important absorption frequencies of different class of organic compounds- hydrocarbons, alcohols, thiols, carbonyl compounds, amines,nitriles.

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

^{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, leaning effect, fluxional molecules, temperature dependent NMR spectra, first order and non-first order NMRspectra.

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

Simplification of NMR spectra: double resonance, paramagnetic shift reagents, increased field strength, deuterium labelling. NOE spectra, heteronuclear coupling. Introduction to 2D NMR; COSY, HETCOR; HMBC, HMQC spectra.

^{13}C NMR: General considerations, comparison with PMR, Off-resonance and noise decoupled spectra, factors influencing carbon chemical shifts, chemical shifts values of saturated aliphatics, unsaturated aliphatics, carbonyls, and aromatics, α,β,γ effects,γgauche

effect. Introduction to DEPT Spectra.

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

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

References (For Modules 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,NewDelhi,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, SaundersCollege Publishing 1977 (For NMR andEPR,Mossbauer)
8. Gunther, NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry,2/e,John Wiley
9. Ferraro, Nakamoto and Brown, Introductory Raman Spectroscopy, 2/e, Academic Press, 2005.

For Modules 5, 6, 7 & 8

1. Lambert, Organic StructuralSpectroscopy, 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 andApplications, 2/e, Narosa
5. Fleming, Spectroscopic Methods in Organic Chemistry, 6/e,McGraw-Hill
6. P S Kalsi, Spectroscopy of organic compounds, New Age International, 2007
7. William Kemp, Organic Spectroscopy, 3e, Palgrave, 2010

ST. THOMAS' COLLEGE(AUTONOMOUS), THRISSUR

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

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

CO1	Identify the role of metal ions in biological systems.
CO2	Comprehend the significance of enzymes in biological systems.
CO3	Interpret the application of organometallic compounds as catalysts.
CO4	Analyse bonding pattern and stability of organomatallic compounds.
CO5	Predict the reactivity and reactions given by organometallic compounds.
CO6	Predict stability of organometallic compounds using 18-electron rule.

Module 1: Introduction to Organometallic Chemistry (9h)

Historical background. Classification and nomenclature. Alkyls and aryls of main group metals. Organometallic compounds of transition metals. The 18-electron rule, electron counting by neutral atom method and oxidation state method. The 16-electron rule.
Metal carbonyls- Synthesis, structure, bonding and reactions. Nitrosyl, dihydrogen and dinitrogen complexes. Transition metal to carbon multiple bond-metal carbenes and carbines.

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

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

Module 3: Organometallic Reactions and Catalysis (9h)

Organometallic reactions- ligand dissociation and substitution- Oxidative addition and reductive elimination. Insertion reactions involving CO and alkenes. Carbonylation by Collman`s reagent. Electrophilic and Nucleophilic attack on coordinated ligand.
Homogeneous and heterogeneous catalysts. Homogeneous catalysis by organometallic compounds: Hydrogenation by Wilkinson`s catalyst, Hydroformylation, Wacker process, Monsanto acetic acid process, Cativa process and olefin metathesis.
Heterogeneous catalysis by organometalic compounds: Ziegler-Natta polymerizations, Fischer- Tropsch process and water gas shift reaction.

Module 4: Metal Clusters (9h)

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

Module 5: Bioinorganic Chemistry-I (9h)

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

Emergence of bioinorganic chemistry. Coordination sites in biologically important ligands. Ion transport across membranes. Role of alkali metal ions in biological systems. The sodium/potassium pump. Structural role of calcium. Storage and transport of metal ions- ferritin, transferrin and siderophores. Oxygen transport by heme proteins-hemoglobin and myoglobin-structure of the oxygen binding site-nature of heme-dioxygen binding-cooperativity. Hemerythrin and hemocyanin.

Module 6: Bioinorganic Chemistry-II (9h)

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

References

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ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

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

CO1	Understand the oxidation reactions in organic chemistry.
CO2	Understand various types of polymerization.
CO3	Use of important synthetic reagents for organic reactions.
CO4	Apply the principles of reduction and various coupling reactions in organic synthesis.
CO5	Apply the mechanisms of the different rearrangements and transformations in chemical reactions.
CO6	Analyse natural and artificial supramolecular systems.
CO7	Analyse the strategy of peptide synthesis.

Module 1: Oxidations (9h)
Oxidation of alcohols to carbonyls using DMSO, oxoammonium ions and transition metal oxidants (chromium, manganese, iron, ruthenium). Epoxydation of alkenes by peroxy acids, Sharpless asymmetric epoxidation, Jacobsen epoxidation, dihydroxylation of alkenes using permanganate ion and osmium tetroxide, Sharpless asymmetric dihydroxylation. Allylic oxidation with CrO_3, Pyridine reagent. Oxidative cleavage of alkenes to carbonyls using O_3. Oxidative decarboxylation, Riley reaction, Dess Martin oxidation, Swern oxidation.

Module 2: Reductions (9h)
Catalytic hydrogenation of alkenes and other functional groups (heterogeneous and homogeneous), Noyori asymmetric hydrogenation, hydrogenolysis. Liquid ammonia reduction with alkali metals. Metal hydride reductions. Reduction of carbonyl group with hydrazine, p-tosylhydrazine, diimide and semicarbazide. Clemmensen reduction, Birch reduction. Wolff Kishner reduction, Bouveault Blanc reduction, MPV reduction, hydroboration and its applications, Pinacol coupling, McMurry coupling, Shapiro reaction.

Module 3: Synthetic Reagents (9 h)
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.

Module 4: Chemistry of Polymers (9 h)
Classification of polymers, chain, step, free-radical and ionic polymerizations. Plastics, rubbers and fibers, thermosets and thermoplastics, linear, branched, cross -linked and network polymers, block and graft copolymers.

Natural and synthetic rubbers.

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

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

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

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 supramoleculardevices

Module 6: Molecular Rearrangements and Transformations (9h)

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

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ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

CHE3E01 - SYNTHETIC ORGANIC CHEMISTRY (ELECTIVE) (4 Credits, 54h)

CO1	Understand the chemistry of carbonyl condensation reactions.
CO2	Understand the chemistry of fused and higher ring heterocyclics.
CO3	Understand the basic principle of multistep synthesis.
CO4	Application of metal catalyzed coupling reaction in organic synthesis.
CO5	Application of organometallic and organo-nonmetallic reagents.
CO6	Application of reagents for oxidation reduction reactions.

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

Reagents for oxidation and reduction: Oxone, IBX, PCC, potassium permanganate, 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.

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

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

Module 3: Chemistry of Carbonyl Compounds (9h)

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

Module- 4. Coupling Reactions (9h)

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

Module 5: Multi step Synthesis and Retrosynthesis (9h)

Multi step Synthesis**:** Synthetic analysis and planning, Target selection, Elements of a Synthesis (Reaction methods, reagents, catalysts, solvents, protective groups for hydroxyl, amino, Carbonyl and carboxylic acids, activating groups, leaving groups synthesis and synthetic equivalents. Types of selectivities (Chemo, regio, stereo selectivities) synthetic planning illustrated bysimple molecules.Synthesis of longifolene, Corey lactone, Djerassi Prelog lactone.

Introduction to retrosynthetic analysis: 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.

Module 6: Heterocyclics (9h)
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).

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ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

CHE3E02 - COMPUTATIONAL CHEMISTRY (ELECTIVE) (4credits, 54h)

CO1	Conceptual understanding of the laws of quantum mechanics necessary for the description of atoms and molecules and their chemical reaction
CO2	Identify and explain the main similarities and differences between theoretical approaches such as HF (Hartree-Fock), DFT (Density Functional Theory)and force field methods.
CO3	Describe advantages / disadvantages for simulating/modelling various scientific problems.
CO4	Choose the appropriate method in terms of applicability, accuracy, and economy for the calculation of a given chemical problem
CO5	Apply quantitative techniques and computational methods in the analysis of chemistry and chemical problems

Module 1: Introduction to Computational Chemistry (9 h)

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

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

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

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

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

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

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

MODULE 5: Density Functional Methods (9 h)

Introduction to density matrices, N-reprentability & V-represetability problems, Hohenberg

– Kohn theorems, Kohn-Sham orbitals, Exchange correlation functionals– Thomas-Fermi-Dirac model, Local density approximation, generalised gradient approximation, hybrid functional. Comparison between DFT and HF methods.

MODULE 6: Basis Set Approximation (9 h)

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

References:

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ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

CHE3E03- GREEN AND NANOCHEMISTRY (ELECTIVE)

(4 credits, 54 h)

CO1	Identify alternative synthesis, reagents and reaction conditions
CO2	Identify the structure of carbon clusters and nanostructures
CO3	Implement green Practices
CO4	Analyze the various methods used in the characterisation of nanomaterials

Module 1: Introduction to green chemistry (9h)

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

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

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

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

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

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

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

Cavitation. Inorganic nanomaterials – Typical examples –nano TiO2 / ZnO/CdO/CdS, Organic nanomaterials – examples – Rotaxanes and Catenanes

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

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

Module 6: Carbon Clusters and Nanostructures (9h)

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

References:

For Modules 1, 2 & 3

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For Modules 4, 5 & 6

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ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

CHE4C12- INSTRUMENTAL METHODS OF ANALYSIS (4 Credits, 72 h)

CO1	Measure errors in analytical data
CO2	Understand the principles of analytical procedures in chemistry
CO3	Identify the components of instruments and tools used in chemical analysis
CO4	Interpret the data obtained from analytical instruments.

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

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

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

Gravimetry: **s**olubility product and properties of precipitates-nucleation, growth and aging, co- precipitation and post precipitation, drying and ignition. Inorganic precipitating agents: NH_3, H_2S, H_2SO_4, $(NH_4)_2MoO_4$ and NH_4SCN. Organic precipitating agents: oxine, cupron, cupferron, 1-nitroso-l-naphthol, dithiocarbamates. Titration curves of strong acid, strong base, weak acid, weak base and polyprotic acids. Buffer solutions. Titrations in nonaqueous media. Different solvents and their selection for a titration. Indicators for non- aqueous titrations. Redox titration - cerimetry. Variation of potential during a redox titration, formal potential during a redox titration, Redox indicators. Precipitation titrations, adsorption indicators. Complexometric titrations: Types of EDTA titrations (direct, back, replacement, alkalimetric and exchange reactions), masking and demasking agents, selective demasking, metal ion indicators - murexide, eriochrome black T, Patton and Reeder's indicators, bromopyrogallol red, xylenol orange, variamine blue.

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

Three electrode cell, Potentiostat, Galvanostat, indicator electrodes.Ion-selective electrodes, glass electrode and applications in pH measurements. Polarography: micro electrode and their specialities, techniques of improving detection limit, ac, pulse, differential pulse, square wave polarographic techniques. Cyclic voltammetry: cyclic voltammogram, concentration profile, half-peak potential, peak current, Randles-Sevcik equation, reversible, quasi reversible and irreversible systems. Classification of electrochemical reaction mechanisms,limitations of CV, acceptable sweep rate ranges of CV. Impedance spectroscopy: Real and imaginary impedance, Impedance of a Capacitor in Series with a Resistor, Cole-Cole plot, Equivalent circuit of electrochemical interface, Applications of impedance spectroscopy to electrode processes.

Module 4: Electro Analytical Methods II (9h)

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

Module 5: Optical Methods - I (9 h)

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

Module 6: Optical Methods - II (9 h)

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

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

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

Module 8: Chromatography (9 h)

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

References:

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ST. THOMAS'COLLEGE(AUTONOMOUS), THRISSUR

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

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

CO1	Identify the ingredients of perfumes.
CO2	Enable to distinguish products of fractional distillation of crude oil.
CO3	Analyse petroleum fuels and its quality standards.
CO4	Analyse the composition of crude petroleum.
CO5	Analyse the uses and purification of petroleum products.
CO6	Analyse the role of chemicals as cosmetics.

Module 1: Introduction to Petrochemistry (9h)

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

Module 2: Hydrocarbons from Petroleum (9h)

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

Module 3: Industrial Organic Synthesis (9h)

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

Module 4: Composition of Petroleum Crude (9h)

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

Module 5: Distillation of Crude Petroleum (9h)

Preparation of petroleum for processing. Destruction of petroleum emulsion. Electric desalting plants. Fundamentals of preliminary distillation. Methods of petroleum distillation. Distillation of crude petroleum. Treatment of the residual liquid processing of liquid fuels such as petroleum and petroleum products. Petroleum processing equipments. Storage tanks.

Rectification columns. Cap tray or bubble tray columns. Heat exchange apparatus. Steam space heaters or boilers. Condensers. Pipe furnaces. Pipelines. Fitting Compressors and pumps.

Module 6: Petroleum Products (9h)

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

Module 7: Purification of Petroleum Products (9h)

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

Module 8: Perfumes and Cosmetics (9h)

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

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

Cosmetics: Economics and Advertising.

References:

1. B. K. Sharma, Industrial Chemistry, Goel Publication,Goa.
2. N. K. Sinha, Petroleum Refining andpetrochemicals.
3. John W. Hill, Chemistry for Changing times, SurjeetPublication.
4. UttamRayChaudhuri,“FundamentalsofPetroleumandPetrochemicalEngineering”, 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

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER IV
CHE4E05 - INDUSTRIAL CATALYSIS (ELECTIVE) (4 Credits, 72h)

CO1	Appreciate the importance of catalysis in industrial processes
CO2	Understand the fundamentals principles of catalysis and kinetics
CO3	Understand methods of preparation of catalysts
CO4	Understand the methods of characterization of catalysts
CO5	Analyze the mechanism of catalyzed chemical reactions

Module 1: Introduction to Adsorption process (9h)

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

Module 2: Kinetics and Catalysis (9h)

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

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.

Module 3: Catalyst - Preparative Methods (9h)

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

Module 4: Deactivation of Catalysts (9h)

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

References:

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

MODULE 5: Phase Transfer Catalysis (9h)

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

MODULE 6: Biocatalysis (9h)

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

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.

MODULE 7: Industrial Catalysis-1 (9h)

Oil based chemistry. Catalytic reforming. Catalytic cracking. Paraffin cracking. Naphthenic cracking. Aromatic hydrocarbon cracking. Isomerization. Hydrotreatment.

Hydrodesulphurization. Hydrocracking. Steam cracking. Hydrocarbons from synthesis gas. Fisher-Tropsch process. Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

MODULE 8: Industrial Catalysis-II (9h)

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

References:

1. G. Ertl, H. Knozinger and J. Weitkamp, "Handbook of Heterogeneous Catalysis" Vol 1-5, Wiley-VCH, Weinheim, 1997.
2. R.J. Farrauto and C.H. Bartholomew, "Fundamentals of Industrial 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.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

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

CO1	Introduce synthetic route of polymers.
CO2	Understand the structure and basic concepts of various dyes and supramolecules.
CO3	Understand the mechanism of polymerization.
CO4	Understand various constituents of natural products.
CO5	Analyse the structure of alkaloids and anthocyanins.
CO6	Analyse the properties of polymers.
CO7	Apply various methods for characterization of polymer.
CO8	Apply the structure elucidation strategy of steroids and terpenoids.

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

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

MODULE 2: Terpenoids and Steroids (9 h)

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

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

MODULE 3: Alkaloids and Anthocyanins (9 h)

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

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

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

References:
1. M. B. Smith, Organic Synthesis, 3/e, Academic Press, 2011.
2. F. A. Carey and R. J. Sundberg: Advanced Organic Chemistry (part B), 3rd ed., Plenum Press.
3. T.W. G. Solomons: Fundamentals of Organic Chemistry, 5th ed., 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, OxfordUniversity Press
8. N. R. Krishnaswamy: Chemistry of Natural Products; A Unified Approach, Universities Press
9. R. J. Simmonds: Chemistry of Biomolecules: An Introduction,RSC
10. R. O. C. Norman: Principles of Organic Synthesis, 3nd ed., CRC Press,1998.
11. J. M. Lehn, SupramolecularChemistry

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

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

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

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

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

Polymer Solutions. Treatment of dilute solution data. Thermodynamics. Flory-Huggins equation.

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

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

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

References:

1. F.W. Billmayer. Textbook of Polymer Science. 3rd Edn, Wiley. N.Y.1991.
2. G. Odiyan, Principles of Polymerisation, 4/e, Wiley,2004.
3. V.R. Gowriker and Others, Polymer Science, Wiley 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.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

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

CO1	Differentiate between ceramics, ferroelectrics and piezoelectric materials.
CO2	Understand theories of superconductivity.
CO3	Understand Ceramic matrix composite materials
CO4	Evaluate methods to test materials
CO5	Evaluate use of different plastics based on their structure and properties.
CO6	Evaluate Micro structural features of fracture.
CO7	Apply sol-gel techniques to synthesize nano-materials.
CO8	Predict material behavior using phase diagrams.

Module 1: Introduction to Material Science (9h)

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

Module 2: Ceramic Materials (9h)

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

Module 3: Nanomaterials and Nanotechnology (9h)

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

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

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

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

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

Module 6: Some Special Polymers (9h)

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

Module 7: Composite Materials (9h)

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

Module 8: Fracture Mechanics (9h)

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

References:

1. W.D. Eingery, H.K. Dowen and R.D. Uhlman, Introduction to Ceramics, 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. R.J. Young, Introduction to Polymer Science, John Wiley andSons.
11. V.R. Gowriker and Others, Polymer Science, Wiley EasternLtd.
12. H. Ulrich, Introduction to Industrial Polymers, Hansen Publishers,1982.
13. F.R. Jones, Handbook of Polymer Fibre Composites, Longman Scientific andTech.
14. K.K. Chowla, Composite Materials, Springer-Verlag, NY,1987.

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

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

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

CO1	Aware of fundamental principles of organometallic chemistry
CO2	Understand the types of reactions and their mechanisms to explore the efficient catalytic processes
CO3	Understand the applications of organometallic homogeneous catalysis
CO4	Predict the role of organometallic catalysts in specific transformations
CO5	Analyze the difference in reactivity of simple organometallic compounds to those of different organometallic polymers

MODULE 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.

MODULE 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.

MODULE 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.

MODULE IV (9h)

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

MODULE V (9h)

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

MODULE VI (9h)

Organometallic reactions. SN^2 Reactions, Radical Mechanisms, Ionic Mechanisms, σ-Bond Metathesis, Oxidative Coupling and Reductive decoupling. Reactions involving CO, Insertions Involving Alkenes, Other Insertions, α, β, γ and δ Elimination, Deinsertion and Nucleophilic and electrophilic attack on coordinated ligand.

MODULE VII (9h)

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

MODULE VIII (9h)

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

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, WileyInterscience.
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.

ST. THOMAS'COLLEGE(AUTONOMOUS), THRISSUR
M.Sc. CHEMISTRY – SEMESTER III & IV

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

CO1	Enable the students to enhance analytical skills.
CO2	Acquire skills in inorganic preparations.
CO3	Appreciate the basic concepts of inter group separation.
CO4	Analyse systematically mixtures containing four cations.
CO5	Apply the principles behind gravimetry to do quantitative analysis.
CO6	Apply the principles behind colorimetry to perform quantitative analysis.

Module 1: Estimation of ions in mixture

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

Module 2: Colorimetric Estimations

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

Module 3: Ion Exchange Methods

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

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

References:

1. Vogel's Text Book of QualitativeInorganic Analysis.
2. I.M. Kolthoff and E.A. Sanderson, QuantitativeChemical Analysis.
3. D.A. Adams and J.B. Rayner, Advanced Practical Inorganic Chemistry.
4. W.G.Palmer, ExperimentalInorganicChemistry.
5. G. Brauer, Hand book of Preparative Inorganic Chemistry.

ST. THOMAS'COLLEGE(AUTONOMOUS), THRISSUR

M.Sc. CHEMISTRY – SEMESTER III & IV

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

CO1	Identify various food colours.
CO2	Determine the purity of organic compounds by chromatographic methods.
CO3	Understand common methods of extraction of natural products.
CO4	Analyse organic compounds by quantitative methods.
CO5	Apply the principle of colourimetry to organic compounds.

Module 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, cholesterol, estimation of amino group, phenolic group and esters. Colourimetric estimations: Vitamins (Ascorbic acid), Drugs – sulpha drug (Sulpha diazine, sulphaguanidine), Antibiotics – Pencillin, Stroptomycin.

References:

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

Module 2: Extractions

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

Module 3: Chromatograhy

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

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

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

Pesticides and herbicides: Oragonochlorine pesticides organo phosphates and carbamate pesticides, Herbicides.
Plant growth stimulants: Indole acetic acid.

References:

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

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

M.Sc. CHEMISTRY – SEMESTER III & IV

CHE3L09 & CHE4L12 – PHYSICAL CHEMISTRY PRACTICALS– III & IV

(3 Credits)

CO1	Determine phase diagram of a ternary liquid system
CO2	Determine specific reaction rate
CO3	Determine surface area of adsorbent
CO4	Determine molecular mass of a solute using depression in freezing point of a liquid solvent
CO5	Determination of specific and molar optical rotations of monosaccharides
CO6	Apply HF/6-31G level of theory to determine various physical constants

SECTION A

Module 1: Chemical Kinetics (4 experiments)

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

Module 2: Adsorption (3 experiments)

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

Module 3: Phase Equilibria (2 experiments)

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

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

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

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

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

4. Study of the reaction $2Kl + Hgl_2 \rightarrow .K_2Hgl_4$ and determination of the concentration of the given KI solution.

Module 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

Module 6: Spectrophotometry (3 experiments)

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

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

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

References:

1. A. Finlay and J.A. Kitchener, Practical Physical Chemistry,Longman.
2. F. Daniels and J.H. Mathews, Experimental Physical Chemistry,Longman.
3. A.H. James, Practical Physical Chemistry, J.A. Churchill 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.

Module 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_2O using the Hartree- Fock method (3-21G, 6-31G, 6-31+G, 6-31+G* basis sets can be used).
6. Computation of the energy of HOMO and LUMO of formaldehyde and ethylene

at the HF/6-31G level of theory.

7. Effect of substituent (F & Cl) on the geometric parameters (like C-C bond length) of ethylene at the HF/6-31G level of theory.
8. Comparison of stability of cis-planar and trans-planar conformers of H_2O_2 at the HF/6- 31G level of theory.
9. Comparison of stability of cis- and trans- isomers of difluoroethylene at the HF/6-31G* level of theory.
10. Computation of the frequencies of normal modes of vibration of molecules like H_2O, NH_3 and CO_2 at 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. http://classic.chem.msu.su/gran/gamess/inde

MODEL QUESTIONPAPERS

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

First Semester M. Sc. Chemistry Examination

CHE1C01 – QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

Time: 3 hrs **Maximum weight: 30**

Section A

(Answer *any 8* questions. Each question carries 1 weightage)

1. Show that e^{ikx} is a momentum eigen state. Draw the real part of the wave function.
2. Evaluate $\left[\widehat{\frac{d}{dx}}, \hat{x}\right]$.
3. Distinguish between: stationary state, energy eigen state, bound state, and unbound state.
4. Illustrate the correspondence principle, in the case of particle in 1D box and 1D quantum harmonic oscillator.
5. Solve the Φ equation for hydrogen atom and find the normalization constant.
6. Draw the polar plot of ψ_{310} of hydrogen atom schematically in yz plane and mark the parts.
7. Write the Slater determinant for Li atom.
8. How is STO constructed?
9. State the four possible normalized spin eigen functions for a two-electron system.
10. State any four key words used in Gaussian input file, with the corresponding out comes.
11. What is electron correlation? Explain its significance.
12. Distinguish between *ab initio* and semi empirical methods. **(8 X 1 = 8 weightage)**

Section B

(Answer *any 4* questions. Each question carries 3 weightage)

13. Calculate the probability of finding a particle between L/4 and L/2 in a 1D box of length L. The particle is in the ground state.
14. Starting with the definition; $\frac{d\langle\hat{p}_x\rangle}{dt} = \frac{i}{\hbar}\langle[\widehat{H}, \hat{p}_x]\rangle$, show that linear momentum is conserved for a particle in an infinite square-well.
15. Write the Schrodinger wave equation for hydrogen atom in spherical polar coordinates and obtain the three independent equations in r, θ and φ by variables separation.
16. Illustrate variation method using a trial function $\phi = x\,(a - x)$, for the particle in one dimensional box.
17. Briefly describe the classification of basis sets.
18. Write the Z-matrix for formaldehyde and water.
19. Explain the principle used in molecular mechanics method. **(4 X 3 = 12 weightage)**

Section C

(Answer *any 2* questions. Each question carries 5 weightage)

20. Using the normalized wave function for the ground state of 1D quantum harmonic oscillator, show that the value of uncertainty in position and momentum in the ground state is exactly $\frac{\hbar}{2}$.
21. Derive the expression for the energy of a 3D quantum rigid rotator.
22. Illustrate the perturbation method using the example of helium atom.
23. Briefly discuss the HF-SCF method to solve many electron atoms.

(2 X 5 = 10 weightage)

Module wise Weightage distribution

Module	**Weightage**
Module 1	6
Module 2	9
Module 3	5
Module 4	5
Module 5	8
Module 6	7
Module 7	6
Module 8	7

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

First Semester M. Sc. Chemistry Examination

CHE1C02 - ELEMENTARY INORGANIC CHEMISTRY

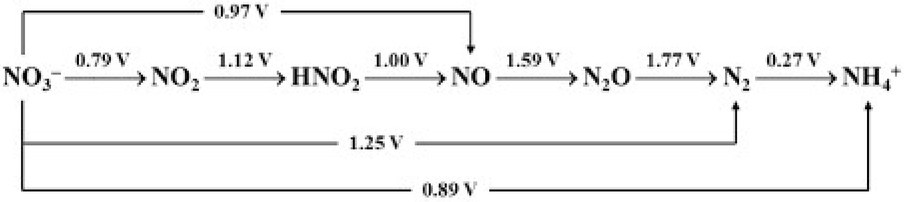
Time: 3 hrs Max. Weight: 30

Section A

*Answer any **eight** questions.*

Each question carries **1** *weightage.*

1. What are super acids? Explain using an example.
2. Boron behaves more like Silicon rather than Aluminum. Why?
3. What happens when vapours of S_4N_4 are a) passes through silver wool at 250°C. b) condensed on glass surface at 10-30°C?
4. What are interstitial carbides? Give an example.
5. The Latimer diagram for nitrogen oxides in given below. Is NO stable with respect to disproportionation under standard conditions at 25°C? Give reason.



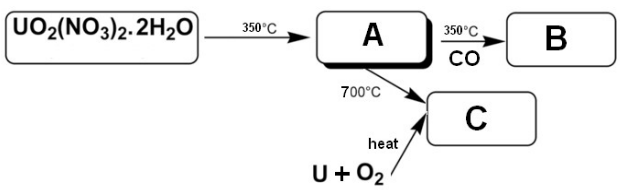
6. For Eu^{3+} the calculated (0 BM) magnetic moment is lower than observed magnetic moment (3.4-3.6 BM) at room temperature. Explain
7. Explain the amphoteric nature of SO_2.
8. Is CaO an acid or base? Explain based on Lux-Flood theory.
9. Explain why HNO_3 behaves as a base in HF?
10. Describe the use of zeolites as water softeners.
11. Why Ce^{3+} is colourless while Ce^{4+} exhibits orange-red color?
12. What makes $_{82}Pb^{208}$ the most stable isotope of lead.

Section B

*Answer any **four** questions.*

Each question carries **3** *weightage.*

13. Derive the Styx code for B_4H_{10}.
14. **X** is the most stable phosphorus sulphide which upon reaction with iodine gives two isomers **Y** and **Z.** **Y** and **Z** upon treatment with $[(CH_3)_3Sn]_2S$ result in α-P_4S_4 and β-P_4S_4. i) Identify **X**, **Y** and **Z**. ii) Draw the structures of α-P_4S_4 and β-P_4S_4.
15. What are the structural features of orthosilicates, pyrosilicates and cyclic silicates which make them differ from each other.
16. Using elligham diagram explain how carbon can be used as a good reducing agent.
17. Uranyl nitrate dehydrate on heating at 350 °C yields an oxide **A**. Oxide **A** can form two other oxides **B** and **C**. Oxide **C** can also be prepared by heating uranium with oxygen. Identify **A**, **B** and **C**.



18. i) Calculate the mass defect and binding energy for the nuclide $_5B^{10}$ where the mass of $_5B^{10}$ atom = 10.0129 amu; mass of proton= 1.007276 amu and mass of neutron= 1.008665 amu.

ii) Complete the following equations by adding the missing species:

a. $^{27}_{13}Al + ^{4}_{2}He \longrightarrow ? + ^{1}_{0}n$

b. $^{239}_{94}Pu + ? \longrightarrow ^{242}_{96}Cm + ^{1}_{0}n$

c. $^{14}_{7}N + ^{4}_{2}He \longrightarrow ? + ^{1}_{1}H$

d. $^{235}_{92}U \longrightarrow ? + ^{135}_{55}Cs + 4\,^{1}_{0}n$

19. Discuss any three methods for Synthesis of nanostructures.

Section C

*Answer any **two** questions.*

*Each question carries **5** weightage.*

20. i) Why is Borazine called inorganic benzene? Using suitable examples compare its reactivity with benzene.

ii) Explain Wade's rule. Using Wade's rules predict the structure of B_6H_{10}. (3+2)

21. Explain HSAB principle and its applications. (2+3)

22. i) How does the shell model explain the structure of nucleus?

ii) Discuss the methods for Detection and measurement of radiation. (1+4)

23. i) Identify any four methods to characterize TiO_2 nanoparticles. What is the information obtained from each technique?

ii) Discuss the biomedical applications of nanoparticles. (2+3)

Module wise Weightage distribution

Module	Weightage
Module 1	9
Module 2	9
Module 3	9
Module 4	9
Module 5	9
Module 6	8

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

First Semester M. Sc. Chemistry Examination

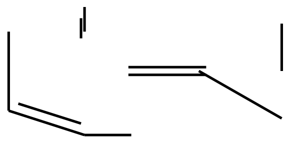
CHE1C03 - STRUCTURE, AND REACTIVITY OF ORGANIC COMPOUNDS

Time: 3 hrs **Maximum weight: 30**

I. Answer any eight of the following questions: (8 x 1 = 8 Weightage)

1. Explain the dipolemoment of 1,2 dichloro ethane increases with temperature.
2. Write Taft equation and explain the terms involved.
3. Draw the structures of the followingmolecules:

   (a) 2R, 3Rtartaricacid (b) Z-3-methyl-2pentene
4. Draw the conformations of cis and trans decaline. Which is the mobile one? Why?
5. Explain why pK_a value for cyclopentadiene is 15 where as it is 36 forcycloheptatriene.
6. Illustrate how the HCl elimination reaction of menthyl and neomenthyl chlorides differ andwhy.
7. Between trans -1,2 dimethyl cyclohexane and cis 1,2 dimethyl cyclohexane, which is more stable andwhy?
8. Discuss the criteria for optical activity in biphenyls.
9. State and explain Cramsrule.
10. Explain the term 'Chiral pool'. What is itsimportance?
11. The following hydrocarbon displays very high dipole moment. Explain.

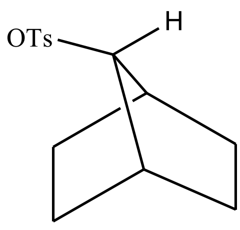


12. Using a Fischer Projection of phenyl acetaldehyde, Identify its Pro-R and Pro-S hydrogens.

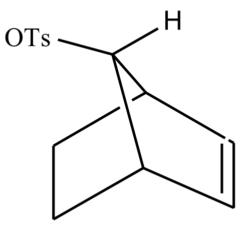
II. Answer any Four of the following questions: (4 x 3 = 12 Weightage)

13. What are chiral auxiliaries? What are the criteria for choosing an effective chiral auxiliary? Illustrate the use of camphor derivative as chiral auxiliaries in Diels – Alder reaction.
14. What is Hammet acidity function? How is it determined?
15. Discuss the optical isomerism exhibited by nitrogen and sulphur compounds.
16. Discuss the effect of conformation on S_N1 and S_N2 reactions of equatorial leaving groups in flexible and rigid cyclohexanes.
17. Comment on the rate of acetolysis of the following compounds:

(a)



(b)



18. Write a note on the aromaticity of any two annulenes. Explain how NMR spectroscopy is useful in establishing that these molecules are aromatic.

19. Describe the conformers and their stability of (a) n-Butane; (b) Ethylene glycol and (c) Acetaldehyde.

III. Answer any two of the following questions (2 x 5 = 10 Weightage)

20. (a) CrO_3 oxidation of cyclohexanols with axial and equatorial OH groups.

(b) Discuss pyrolytic elimination of esters.

21. Discuss the stereochemistry of aldoximes and ketoximes with an example.

22. Discuss the effects of hydrogen bonding (intra- and intermolecular) on boiling point, acidity, basicity and stability of conformational isomers. Use appropriate examples.

23. (a) Discuss linear free energy relationship in Hammett and Taft equation for total polar effects.

(b) What is Hammett acidity function?

Module wise Weightage distribution

Module	Weightage
Module 1	10
Module 2	12
Module 3	5
Module 4	10
Module 5	10
Module 6	6

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

First Semester M. Sc. Chemistry Examination

CHE1C04 – THERMODYNAMICS, KINETICS AND CATALYSIS

Time: 3 hrs **Maximum weight: 30**

Section A

(Answer *any 8* questions. Each question carries 1 weightage)

1. What is meant by encounter in chemical dynamics?
2. Distinguish between diffusion controlled and activation controlled reactions.
3. What is chain retardation? Give an example.
4. Write the London equation and explain the terms.
5. Define Fugacity and Activity.
6. Explain residual entropy with suitable examples.
7. Give Glansdorf-Pregogine equation and explain terms.
8. Explain the term excess enthalpy.
9. The slope and intercept for Langmuir adsorption process are 0.55 Pacm^{-3} and 0.525 X 10^{-3} cm^{-3}. Find the value of adsorption coefficient.
10. How can we determine the surface acidity?
11. Briefly explain the various adsorption isotherms.
12. Spontaneous adsorption is always exothermic. Explain. **(8 X 1 = 8 weightage)**

Section B

(Answer *any 4* questions. Each question carries 3 weightage)

13. Derive the Lindemann's kinetics for unimolecular reactions. How does the order of the reaction vary with pressure?
14. Define phenomenological coefficients. Show that direct coefficients always dominate indirect coefficients.
15. Write a note on the determination of the surface area and pore structure of adsorbents.
16. Distinguish between attractive and repulsive potential energy surfaces.
17. Define chemical potential. Discuss its variation with temperature and pressure.
18. Discuss Langmuir-Hinshelwood and Eley-Rideal mechanism for the oxidation of CO.
19. Derive the relation between rate constant of a reaction in solution and ionic strength of the medium.

(4 X 3 = 12 weightage)

Section C

(Answer *any 2* questions. Each question carries 5 weightage)

20. Discuss the decomposition of acetaldehyde and derive the rte laws.
21. Derive the BET equation.
22. Explain the specific reaction rate of energized molecules is an energy dependent step by RRK treatment.
23. Discuss the determination of absolute entropies of solids, liquids and gases in the context of third law of thermodynamics. **(2 x 5 = 10 weightage)**

Module wise Weightage distribution

Module	Weightage
Module 1	10

Module 2	5
Module 3	11
Module 4	12
Module 5	10
Module 6	5

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

Second Semester M. Sc. Chemistry Examination

CHE2C05 - GROUP THEORY and CHEMICAL BONDING

Time: 3 hrs **Maximum weight: 30**

Section A

(Answer *any 8* questions. Each question carries 1 weightage)

1. What is cyclic group. Write one example.
2. List the symmetry elements associated with a Td molecule.
3. Generate a matrix for S_3 operation.
4. What do the Mulliken symbols B_{2u} and A_{1g} signify?
5. Explain the term non-vanishing integral. Write one example.
6. Find $A_2 x B_2$ in C_{2V} point group.
7. What do you mean by projection operator?
8. Distinguish between SAGO and SALC .
9. Obtain the term symbol for oxygen molecule in the ground state.
10. Explain Born – Oppenheimer approximation.
11. Draw Frost -Hückel circle and represent the energy level (α-2β) on benzene.
12. Write the Hückel theory secular equation for ethylene. What values of E permit solution of the secular equation? **(8 x 1 = 8 weightage)**

Section B

(Answer *any 4* questions. Each question carries 3 weightage)

13. Show that the symmetry operations E, $C_{2(z)}$, σ_{xy} and i form a mathematical group.
14. State GOT and derive C_{4v} character table.
15. State mutual exclusion principle and rationalize using group theory.
16. Construct the Molecular orbitals of HCHO molecule.
17. Construct the SALCs of the sigma bonds of NH_3 molecule.
18. Briefly discuss the importance of correlation diagram.
19. Construct the HMOs for butadiene and deduce the delocalization energy.

(4 x 3 = 12 weightage)

Section C

(Answer *any 2* questions. Each question carries 5 weightage)

20. Find IR and Raman active vibrations in NH_3. Use C3v character table (below)
21. Construct the hybrid orbitals of BF_3 molecule using the method of SALCs.
22. Compare and contrast MO theory and VB theory with suitable example.
23. Discuss the quantum mechanical treatment of sp^3 hybridisation.

(2 x 5 = 10 weightage)

Module wise Weightage distribution

Module	Weightage
Module 1	5
Module 2	8
Module 3	10
Module 4	10
Module 5	10
Module 6	10

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

Second Semester M. Sc. Chemistry Examination

CHE2C06 - CO-ORDINATION CHEMISTRY

Time: 3 hrs Max. Weight: 30

Section A

*Answer any **eight** questions.*

*Each question carries **1** weightage.*

13. Explain Chelate effect.
14. What is the importance of Marcus equation?
15. $Ni(CN)_4$ is square planar, but $Ni(H_2O)_6$ is octahedral in shape. Give reason.
16. Find the ground state term symbol for Fe^{2+} and Cr^{3+}.
17. Comment on the structure and stereoisomerism exhibited by bis(benzoylacetonate)Be(II).
18. Distinguish between prompt and delayed photochemical reactions.
19. Define EAN. Calculate the EAN of Cr(III) in $[Cr(NH3)_6]Cl_3$.
20. Explain temperature independent paramagnetism with example.
21. The rate constant for electron transfer between $[Fe(H_2O)_6]^{2+}$ and $[Fe(OH)(H_2O)_5]^{2+}$ is reduced to 50% on changing the reaction medium from H_2O to D_2O. Give reason.
22. Define photosubstitution and state Adamsons rules on photosubstitution.
23. State the selection rules for relative intensities of absorption spectra of metal complexes.
24. Differentiate between aquation and base hydrolysis in octahedral substitution reactions of metal complexes. (8 x 1 = 8)

Section B

*Answer any **four** questions.*

*Each question carries **3** weightage.*

24. Distinguish between macrocyclic effect and template effect with examples.
25. Briefly discuss the applications of Mossbauer spectroscopy to iron and tin complexes.
26. Explain the substitution reactions in square planar complexes.
27. Explain briefly the stereoisomerism exhibited by 4 and 6 coordinated complexes.
28. Distinguish between Tanabe Sugano diagrams and Orgel diagrams.
29. What is the effect of pi bonding ligands in the MO diagram of octahedral complexes? Explain with examples.
30. What are CT spectra? Discuss the different type of charge transfer bands and their origin.

(4 x 3 = 12)

Section C

*Answer any **one** question.*

*Each question carries **5** weightage.*

31. Describe the mechanism of electron transfer reactions in metal complexes, bringing out the various factors which affect the reactions.

32. Give an account of the applications of IR spectra in the structural elucidation of metal complexes.

33. (a) Explain outer sphere and inner sphere mechanism with examples.

(b) Discuss photochemical reactions of metal complexes.

34. (a) What are the major assumptions of crystal field theory of complexes? Explain the splitting pattern in octahedral, tetragonal, tetrahedral and square planar complexes with necessary diagrams.

b) Briefly explain Jahn teller effect and its consequences. (2 x 5 = 10)

Module wise Weightage distribution

Module	Weightage
Module 1	9
Module 2	9
Module 3	9
Module 4	8
Module 5	9
Module 6	9

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

Second Semester M. Sc. Chemistry Examination

CHE2C07 - REACTION MECHANISM IN ORGANIC CHEMISTRY

Time: 3 hrs **Maximum weight: 30**

I. Answer any eight of the following questions: (8 x 1 = 8 Weightage)

1. What is the significance of Barton reaction?
2. What is *cine* substitution?
3. What are ambident nucleophiles? Give an example.
4. What is Paterno-Buchi reaction?
5. What is Emde degradation?
6. What are anthocyanins?
7. Write a short note on E1CB Mechanism.
8. Draw the structure of reserpine.
9. Explain photosensitization and quenching
10. Write the mechanism of Norrish type II reaction
11. Write a short note on pyrolytic syn elimination
12. Explain Di-methane rearrangement

II. Answer any Four of the following questions: (4 x 3 = 12 Weightage)

13. Discuss the structure and formation of triplet and singlet carbenes.
14. Write a short note on Jablonski diagram.
15. Discuss the factors which affect elimination reactions.
16. Illustrate the stereochemistry and regioselectivity of Diels-Alder reaction.
17. Discuss the mechanistic features of ester hydrolysis.
18. Write a note on S_E2 and S_Ei reactions.
19. Complete the following reaction with a suitable mechanism

III. Write essays on any two of the following: (2 x 5= 10 Weightage)

20. Derive the selection rules for sigmatropic migration of alkyl groups using FMO method.
21. Write the mechanism for: (a) Dieckmann condensation (b) Thorpe condensation (c) Prince reaction and (d) Ritter reaction.
22. Explain: (a) SET mechanism (b) E1cB mechanism (c) Benzyne mechanism (d) S_Ni mechanism.
23. Discuss the degradative reactions used for the structure elucidation of alkaloids.

Module wise Weightage distribution

Module	Weightage
Module 1	10
Module 2	8
Module 3	8
Module 4	8
Module 5	11
Module 6	8

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR
Second Semester M. Sc. Chemistry Examination
CHE2C08 - ELECTROCHEMISTRY, SOLID STATE CHEMISTRY AND STATISTICAL THERMODYNAMICS

Time: 3 hrs **Maximum weight: 30**

Section A

(Answer *any 8* questions. Each question carries 1 weightage)

1. Explain Density of States.
2. Comment on Ni-Cd cells.
3. What is meant by rotational temperature?
4. Explain the significance of partition function.
5. Distinguish between Bosons and Fermions.
6. Write Hermann-Maugin symbol for: (a) D_{2d} (b) C_{4h}.
7. List the various Bravais lattices under cubical symmetry.
8. Account for the anomalous heat capacity of H_2.
9. Write Schoenflies notation for (a) mmm (b) 222.
10. What is concentration polarization?
11. Define Fermi level. Explain its significance.
12. What is Brillouin zone? **(8 x 1 = 8 weightage)**

Section B

(Answer *any 4* questions. Each question carries 3 weightage)

13. Calculate mean ionic activity coefficient of 0.01 molal $LaCl_3$ in water at 25^0 C. The A value in the Debye Huckel equation is 0.509.
14. How can you determine individual electrode over voltage?
15. Draw stereographic projection for point groups under monoclinic system
16. Explain the term glide plane and screw axis.
17. Write short note on Band–Band Transitions.
18. (a) What are the electrode reactions in direct methanol fuel cells? (b) What are the advantages of fuel cells.
19. Derive Bose-Einstein distribution law. **(4 x 3 = 12 weightage)**

Section C

(Answer *any 2* questions. Each question carries 5 weightage)

20. Derive Debye Huckel Onsager equation.
21. What is hydrogen overvoltage? Discuss the various theories of hydrogen overvoltage.
22. (a) Derive an equation for the translational partition function for a delocalized system containing N particles.

(b) Deduce an expression for internal energy and equilibrium constant in terms of partition function.

23. Discuss the Debye's theory of heat capacity of solids. **(2 x 5 = 10 weightage)**

Module wise Weightage distribution

Module	**Weightage**
Module 1	12
Module 2	9
Module 3	9
Module 4	6
Module 5	7
Module 6	10

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

Third Semester M. Sc. Chemistry Examination

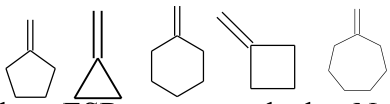
CHE1C04 – THERMODYNAMICS, KINETICS AND CATALYSIS

Time: 3 hrs **Maximum weight: 30**

Section- A

(Answer any eight questions. Each question carries a weight of 1)

1. Write down the total number of signals obtainable in PMR spectra of the following molecule : 2R, 3R-2, 3 dibromo pentane, Fumaric acid.
2. What is rule of thirteen in mass spectroscopy?
3. Explain the use of UV spectra in distinguishing axial and equatorial confirmations using a suitable example.
4. The rotational constant of $^{14}N_2$is 2cm^{-1}, the $\mu$of incident radiation in raman spectrometer is 20487 cm^{-1}. What is the $\mu$of the first scattered stock line in cm^{-1} of $^{14}N_7$?
5. 4-hydroxybenzoic acid exhibited signals at δ 171, 162, 133, 122 and 116 ppm in its broad band decoupled C^{13}NMR spectrum. Correctly assign the signals.
6. An AX system gave 4 lines at 4.72, 4.6, 1.12, 1.0 ppm away from the TMS using an NMR spectrometer operating at 100MHz. What are the values of J_{AX}(in Hz) and δ_{AX}(in ppm) respectively?
7. Classify each of the following molecules as spherical, symmetrical, and asymmetrical top molecule: CH_4, CH_3Cl, CH_2Cl_2, $CHCl_3$.
8. Explain why in the mass spectrum of bromo benzene, there will be two peaks at m/z156 and 158 of approximately equal intensity.
9. Discuss about rigid rotor model.
10. Why vibrations involving relatively neutral bonds such as C-C, C-H, C=C are Strong Raman scatters while they are weak in IR absorption?
11. Arrange in the decreasing order of olefinic stretching frequency:



12. Which of the following will show ESR spectra and why: N_2, H_2, O_2, Cu^{2+}, Cu^{+}, H.

Section B

(Answer any four questions. Each question carries a weight of 3)

13. Explain how Mossbauer spectroscopy is useful in understanding electronic structure of molecule.
14. State and explain (a)Mc Connell relation, (b) Kramers theorem and (c) Ladder operators
15. An organic compound with 5 carbon atoms gives the following signals in H^1NMR spectrum: δ ppm-0.92(t), 1.6(m), 2.23(s), 2.4(t) its IR spectrum showed a strong absorption band at 1718 cm^{-1}. It gives 5 signals in the C^{13}NMR spectrum. Deduce the structure.
16. Give the detailed account on HMBC, HMQC and DEPT.
17. Predict the proton NMR spectra of the following molecule: t-butyl benzene and 2, 2-dimethyl propanal. Is there any rule for anisotropy in the NMR spectra of these molecules?
18. Explain the principle of 2D NMR. Explain HOMOCOSY and HETROCOSY.

19. (a) The rotational constant of HCl^{35} molecule is 12.18 cm^{-1}. Whereas HCl^{37} is found to be 10.18 cm^{-1}. What will be the ratio of the reduced mass of HCl^{37} to HCl^{35}?

(b) For a diatomic molecule AB, the energy for the rotational transition from J = 0 to J = 1 state is 3.9 cm^{-1}. The energy for the rotational transition from J = 3 to J = 4 state would be?

Section C

(Answer any two questions. Each question carries a weight of 5)

20. (a) Describe various types of coupling and factors influencing coupling constant.

(b) Write briefly on (i) first order nmr spectra (ii)Quadrapole broadening

21. (a) Write on the vibrational rotational spectra of diatomics showing the origin of P branch and R branch of lines.

(b) The equilibrium vibration frequency of the iodine molecule I_2 is 215cm^{-1} and the anharmonicity constant is 0.003; What, at 300K, is the intensity of the hot band relative to that of the fundamental band?

22. (a) Discuss the factors contributing to the position and intensity of electronic absorption bands.

(b) Give the detailed account of the applications of ORD and CD studies on organic molecules.

23. The phyto toxic fungal metabolite Pyrenocine (molecular formula $C_{11}H_{14}O_4$) had IR absorption at 3410, 1710 and 1640 cm^{-1} and an intense UV absorption at 284nm. It possessed H^1NMR signals at δ 1.71(3H, d, J = 5.5Hz), 2.31(3H, s), 2.64(1H, exchanged on shaking with D_2O), 3.86(3H, s), 5.15(1H, d, J = 7Hz), 5.50(1H, s), 5.6(1H, d, J = 15.5Hz of q, J = 5.5Hz) and 5.75(1H, d, J = 15.5Hz of d, J = 7Hz). Irradiation of the signal δ 1.71 collapsed the multiplet at δ 5.60 to a doublet (J = 15.5Hz) and irradiationof the signal at δ 5.15 collapsed the signal at δ 5.75 to a doublet (J = 15.5Hz). The signal at δ 5.15 received NOE enhancements on irradiation of the signal δ 2.31 and 3.86 but the signal at at δ 5.50 only received an enhancement from irradiation at δ 3.86. Suggest a structure for pyrenocine.

Module wise Weightage distribution

Module	Weightage
Module 1	4
Module 2	7
Module 3	7
Module 4	7
Module 5	7
Module 6	7
Module 7	7
Module 8	7

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

Third Semester M. Sc. Chemistry Examination

CHE3C10 - ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY

Time: 3 hrs **Maximum weight: 30**

SECTION A

I. Give short answers to any 8 questions. Each question carries a weight of 1

1. Mention two applications of metal carbine complexes in organic synthesis.
2. What is the significance of 16-electron rule?
3. What is meant by hapticity? What hapticities are possible for 1,4-butadiene? Sketch the interactions.
4. What is the effect of increasing pressure of CO and H_2 on the rate of hydroformylation reactions?
5. Explain the role of co-catalyst in Wacker process.
6. What is the synthetic use of Collmans Reagent?
7. Discuss the pre-requisites for the formation of metal-metal bonds.
8. What is 'cooperativity' and Bohr effect?
9. Discuss the role of transferrin and ferritin in iron metabolism.
10. What electron systems are used in photosynthesis?
11. Explain the role of manganese in photosynthesis.
12. What are cytochromes? Mention its function in biological systems.

SECTION B

II. Answer any 4 questions. Each question carries a weight of 3

13. Give an account of the nature of bonding in metal nitrosyls.
14. Discuss structure and bonding in ferrocene.
15. How zeize's salt is synthesized? Discuss the structure and biological structure.
16. Give an account of Monsanto acetic acid process.
17. What are different types of metal clusters?
18. Give Wade-Mingos-Lauher rules.
19. Differentiate between active transport and passive trqansport across biological membrane.

SECTION C

III. Answer any two questions from the following. Each question carries a weight of 5.

20. Discuss with suitable examples the usefulness of 18-electron rule in predicting the formation and stability of organometallic compounds.
21. With suitable example, explain reductive elimination and oxidative addition reactions catalyzed by organometallic compounds.
22. Discuss the function of sodium- potassium pump in biological system. How does vanadate ions interfere with the action of sodium- potassium pump.
23. Describe the function of Photosystem I and Photosystem II in photosynthetic process. Suggest a synthetic model for photosynthesis.

Module wise Weightage distribution

Module	Weightage
Module 1	10
Module 2	7
Module 3	11
Module 4	7
Module 5	10
Module 6	8

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

Third Semester M. Sc. Chemistry Examination

CHE3C11 - REAGENTS AND TRANSFORMATIONS IN ORGANIC CHEMISTRY

Time: 3 hrs **Maximum weight: 30**

Section A

(Answer any eight questions. Each question carries a weight of 1)

1. What is Swern oxidation?
2. What is Riley reaction?
3. What is MPV reduction?
4. What is McMurry coupling?
5. What are crown ethers?
6. Explain the use of Lindlar catalyst in organic synthesis.
7. What are synthetic rubbers?
8. What do mean by graft copolymers?
9. Give one method for pyridine synthess.
10. What do you mean by molecular recognition?
11. What is Wittig reaction?
12. What is Fries rearrangement?

(8 x 1 = 8)

Section B

(Answer any four questions. Each question carries a weight of 3)

13. Discuss any three methods for oxidation of alcohols to carbonyls.
14. Describe hydroboration and its applications in organic synthesis
15. Explain the use of Baker's yeast in organic synthesis
16. What are protecting groups? Illustrate with examples.
17. Discuss the use of hydrogen bonds in crystal-engineering and molecular recognition.
18. Differentiate between Woodward and Prevost hydroxylation reactions
19. Write the mechanism of Suzuki coupling reaction.

(4 x 3 = 12)

Section C

(Answer any two questions. Each question carries a weight of 5)

20. Write notes on (a) Sharpless asymmetric epoxidation and (b) Jacobsen epoxidation
21. Discuss the primary, secondary and tertiary structure of proteins.
22. Discuss any two methods each for the synthesis of uracil, thymine and guanine.
23. Discuss the rearrangements occurring through carbocation intermediate.

(2 x 5 = 10)

Module wise Weightage distribution

Module	Weightage
Module 1	10
Module 2	5
Module 3	10

Module 4	10
Module 5	10
Module 6	8

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

Third Semester M. Sc. Chemistry Examination

CH3 E01: Synthetic Organic Chemistry

Time: 3 hrs **Maximum weight: 30**

I. Give short answers to any eight of the following questions: (8 x 1 = 10 Weightage)

1. What is Gilman reagent? Mention its application.
2. Write one example which involve phosphorous ylide.
3. What TEMPO oxidation?
4. Give a method for the synthesis of Indole.
5. Write down the selectivity of birch reduction.
6. Explain the mechanism of Prins reaction.
7. Explain the oxidation of organoboranes with suitable examples.
8. Write down applications of tributyl tin hydride.
9. Explain the protection of alcohols as Tetrahydropyranylether & Methoxyethoxymethylether.
10. Give the structure of Vitamin C.
11. Write briefly a note on Benzene Tricarbonyl Chromium.
12. Illustrate the use of leadtetraacetate as oxidant in organic synthesis.

II. Answer any four of the following in paragraph: (4 x 3 = 12 Weightage)

13. Give the synthesis of longifolene.
14. Write a note on disconnection in Retro Synthetic analysis with suitable examples.
15. Discuss the mechanism & synthetic application of Sonogashira cross coupling reaction.
16. Explain the mechanisms of following reaction with suitable examples:

    a) Perkins reaction b) Dieckmann reaction
17. Explain the general methods for the synthesis of the following heterocyclic compounds: Benzofuran b) tetrazole
18. Discuss retrosynthetic analysis of paracetamol from phenol.
19. Give the synthesis & reactions of quinoiline.

III. Write essays on any two of the following: (2 x 5 = 10 Weightage)

20. Enumerate with suitable examples, the synthetic uses of osmium tetroxide, ruthenium tetroxide & molecular oxygen as oxidants.
21. Bring about the mechanisms of the following reactions: (a) Darzen reaction

    (b) Stork-enamine reaction (c) Kumada coupling (d) Heck coupling
22. (a) Describe the salient steps in the synthesis of vitamin C. (b) Explain Wacker & Swern oxidation.
23. a) Write brief note on retrosynthetic analysis with suitable examples. B) Discuss the use of phase transfer reagents.

Module wise Weightage distribution

Module	Weightage
Module 1	9
Module 2	9
Module 3	8
Module 4	9
Module 5	9
Module 6	9

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

Fourth Semester M. Sc. Chemistry Examination

CH4 C12: Instrumental Methods of Analysis

Time: 3 hrs **Maximum weight: 30**

I. Give short answers to any eight of the following questions: (8 x 1 = 8 Weightage)

1. What are the limitations of glass electrode?
2. Explain the variation of potential during redox titration.
3. Discuss the differences between DTA & DSC on thermal methods of analysis.
4. What is the principle of Auger Electron spectroscopy?
5. Write a note on minimization of errors.
6. Give the advantages of coulometric titrations.
7. Mention the applications of isotope dilution analysis.
8. Discuss briefly the nature of indicators on acid-base titrations.
9. Explain organic precipitating agents with suitable examples.
10. What is meant by concentration polarization?
11. What is SEM? Explain.
12. A sample absorbs 30% of the radiation passing through it. Calculate the absorbance.

II. Answer any four of the following in paragraph: (4 x 3 = 12 Weightage)

13. Explain Gel-permeation chromatography.
14. Discuss Amperometric titrations.
15. Explain the terms accuracy & precision. Give the differences between them.
16. What are biosensors? Explain with suitable examples.
17. Discuss the principle & procedure of AFS.
18. Explain briefly principle and application of ESCA.
19. What is thermometric titration?

III. Write essays on any two of the following: (2 x 5 = 10 Weightage)

20. Explain the principle, instrumentation and application of IR spectrophotometry.
21. Discuss the theory & instrumentation of TGA. What are the factors effects on thermal decomposition curve?
22. What are the components of a gas chromatograph? Mention the important application of GC.
23. Discuss the principle, procedure and applications of polarography.

Module wise Weightage distribution

Module	Weightage
Module 1	7
Module 2	7
Module 3	7

Module 4	7
Module 5	7
Module 6	7
Module 7	5
Module 8	6

ST. THOMAS' COLLEGE (AUTONOMOUS), THRISSUR

Fourth Semester M. Sc. Chemistry Examination

CHE4E06 - NATURAL PRODUCTS & POLYMER CHEMISTRY

Time: 3 hrs **Maximum weight: 30**

Section- A

(Answer any eight questions. Each question carries a weight of 1)

1. What are oleoresins?
2. How prostaglandins are classified?
3. Draw the structure of cholesterol.
4. What are anthocyanins?
5. What are chalcones?
6. Draw the structure of β-carotene.
7. What do you mean by Host-Guest relationship in molecular recognition?
8. What do mean by living polymers?
9. Write the Mayo-walling equation and explain its significance.
10. Explain the term glass transition.
11. What are EVA polymers?
12. Explain the structural requisites in polymers with NLO properties

(8 x 1 = 8)

Section B

(Answer any four questions. Each question carries a weight of 3)

13. Describe the synthesis of prostaglandins.
14. Describe the biosynthesis of papaverine.
15. Write short note on phthalocyanines.
16. Discuss with suitable example the ring opening polymerization process.
17. Write a note on coordination polymerization.
18. Briefly discuss the determination of degree of crosslinking in polymers.
19. What are conducting polymers? Discuss its properties with suitable examples.

(4 x 3 = 12)

Section C

(Answer any two questions. Each question carries a weight of 5.)

20. Discuss the general methods of isolation of alkaloids and steroids.
21. Describe the structural elucidation of quinine based on degradative reactions.
22. Describe various polymerization techniques.
23. What are industrial polymers? Discuss the synthesis, structure and applications of any two industrial polymers.

(2 x 5 = 10)

Module wise Weightage distribution

Module	Weightage
Module 1	5
Module 2	5
Module 3	9
Module 4	7
Module 5	9
Module 6	5
Module 7	9
Module 8	4