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#### (Abstract)

MSc Chemistry Programme- Scheme, Syllabus and Pattern of Question papers (Ist and IInd semester only) under Choice Based Credit and Semester System (Outcome Based Education system- OBE ) in Affiliated Colleges with effect from 2023 admissions - Implemented- Orders issued.

# ACAD/ACAD C4/16389/2023

ACADEMIC C SECTION

Dated: 22.08.2023

Read:-1. U.O No. Acad C2/429/2017 Dated 08.09.2020

2. U. O No. Acad C1/21246/2019 Dated 07.12.2020

3 . U.O. No. Acad/C1/21246/2019 dated 16.02.2023 ,

4. U.O. No. Acad/C1/21246/2019 dated 20.04.2023

5. Minutes of the meeting of the CSMC & Conveners of Adhoc committee held on 15.06.2023

6. U.O. No. Acad/C1/21246/2019 dated 09.08.2023

7. Minutes of the Meeting of the Adhoc committee for MSc Chemistry programme held on 10.08.2023

8. Syllabus submitted by the Convenor, Adhoc committee for MSc Chemistry Programme dated 18.08.2023

#### ORDER

1. A Curriculum Syllabus Monitoring Committee comprising the members of the Syndicate was constituted for the Syllabus revision of UG & PG Programmes in Affiliated Colleges, vide paper read (1) above and as per the recommendation of this Committee in its meeting held on 20.11.2020, constitute a sub Committee to prepare the Regulation for PG programmes in Affiliated Colleges vide paper read (2) above.

2. As the reconstitution of Board of Studies of the University is under consideration of the Hon'ble Chancellor, considering the exigency of the matter, Ad hoc Committees were constituted vide paper read (3) above, & it has been modified vide paper read (4) above to revise the Curriculum and Syllabus of PG Programmes in Affiliated Colleges w.e.f 2023-24 academic year.

3. The combined meeting of the Curriculum Syllabus Monitoring Committee & Conveners of Adhoc committee held on 15.06.2023 at syndicate room discussed in detail the draft Regulation, prepared by the Curriculum Syllabus Monitoring Committee, for the PG programmes under Choice Based Credit and Semester System to be implemented in Affiliated Colleges w.e.f 2023 admission and proposed the different phases of Syllabus revision process such as subject wise workshop, vide paper read (5) above.

4. Revised Regulation for PG programmes under Choice Based Credit and Semester System (in OBE-Outcome Based Education System) was approved by the Vice Chancellor on 05.08.2023 and implemented w.e.f 2023 admission vide paper read (6) above.

5. Subsequently, as per the paper read (7) above, the Ad hoc committee for M.Sc Chemistry programme finalized the Scheme, Syllabus and Pattern of question papers of I<sup>st</sup> & II<sup>nd</sup> semester M.Sc Chemistry programme to be implemented w.e.f 2023 admission

6. As per the paper read (8) above, the Convener, Ad hoc committee for M.Sc Chemistry submitted the finalized copy of the Scheme, Syllabus and Pattern of question papers of I<sup>st</sup> & II<sup>nd</sup> semester M.Sc Chemistry programme for implementation w.e.f 2023 admission

7. The Vice Chancellor after considering the matter in detail and in exercise of the powers of the Academic Council conferred under section 11(1) Chapter III of Kannur University Act, 1996 and all other enabling provisions read together with, accorded sanction to implement the Scheme, Syllabus and Pattern of question papers of I<sup>st</sup> & II<sup>nd</sup> semester M.Sc Chemistry programme under Choice Based Credit and Semester System (in OBE- Outcome Based Education System) in Affiliated

# Colleges under the University w.e.f 2023 admission , subject to report to the Academic Council.

8. The Scheme, Syllabus and Pattern of question papers of I<sup>st</sup> and II<sup>nd</sup> semester M.Sc Chemistry programme under Choice Based Credit and Semester System ( in OBE- Outcome Based Education System) in Affiliated Colleges under the University w.e.f 2023 admission is uploaded in the University website

9. Orders are issued accordingly.

Sd/-Sajesh Kottambrath Assistant Registrar1 For REGISTRAR

To:

- 1. Principals of Affiliated Colleges offering MSc Chemistry Programme
  - 2. Convener, Curriculum Syllabus Monitoring Committee.
  - 3. Convener, Ad hoc Committee for M.Sc Chemistry Programme

Copy To: 1. The Examination Branch (Through PA to CE)

2. PS to VC / PA to PVC / PA to R/PA to FO

3. DR / AR 1 (Acad) /All sections of Academic Branch/Computer Programmer 4. SF / DF /FC

5.Web Manager (for uploading on the website)

Forwarded / By Order OFFICER SECTION



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# KANNUR UNIVERSITY

# SYLLABUS

For MSc Programme in CHEMISTRY in affiliated colleges-2023

Syllabus under Choice Based Credit and Semester System with effect from 2023 admission OUTCOME-BASED EDUCATION - SYSTEM (OBE)

2023

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#### **1. PREFACE**

The syllabi of the MSc programme in Chemistry offered in the university's affiliated colleges under the semester system were revised in light of the decision of the Syndicate of Kannur University, Curriculum Syllabus Monitoring Committee, PG Board of Studies and Chemistry (PG) Ad hoc committee meetings, and the revised syllabi are effective from 2023 admission onwards. There are two independent PG programmes in Chemistry for affiliated colleges, namely MSc Chemistry, and M Sc Chemistry with Drug Chemistry Specialization. The ad-hoc committee formed by Kannur University as per order number Acad/C1/21246/2019 dated 10/02/2023, Kannur University, has prepared the revised curriculum and syllabus for both the programmes to be outcome-based by 2023 regulations.

Candidates with bachelor's degrees in Chemistry/Polymer Chemistry with Mathematics and Physics/Computer science as subsidiary subjects are eligible for admission to these courses. Rules regarding minimum marks required for the Bachelor's degree, reservation, etc., will be as laid down by the University from time to time. The coursework shall be by the scheme of valuation and syllabus prescribed.

The Ad hoc Committee acknowledges the support of Dr. Sudheesh S, School of Chemical Sciences, Kannur University, Dr. Retheesh K, Govt. College, Karyavattom as resource persons and teachers of affiliated colleges who participated in the workshops held on 30<sup>th</sup> June 2023 and 5<sup>th</sup> July 2023.

The Ad hoc Committee for MSc Chemistry Syllabus Revision

- Dr. Shibu P V, (Convenor), Assistant Professor Department of Chemistry, Govt. Brennen College, Thalassery
- Dr. Pushpaletha P, HoD & Professor, Department of Chemistry, Government College, Kasaragod
- Dr Jithesh K, Assistant Professor, Department of Chemistry, Sree Narayana College Kannur.
- Dr Sujith K. V, Assistant Professor Department of Chemistry, Payyanur College, Payyanur
- Jaison P K, Assistant Professor, Department of Chemistry, KMM Govt Women's College Kannur
- Dr. Jitha Kunhikrishnan M, Assistant Professor, Department of Chemistry, Sree Narayana College Kannur
- Dr. Keerthi Mohan A, Assistant Professor, Department of Chemistry, Govt College, Kasaragod

#### **POST GRADUATE PROGRAMME IN CHEMISTRY**

# (Syllabus under choice credit-based semester system (OBE) with effect from 2023 admission)

Master of Science in Chemistry is a Post Graduate level course that aims at an advanced level understanding of major concepts, theoretical principles, experimental aspects, and research aptitudes in chemical sciences. The MSc Chemistry program is designed to provide students with advanced knowledge and skills in various branches of chemistry. Following the principles of Outcome-Based Education (OBE), the program aims to equip students with the necessary theoretical foundation, practical laboratory skills, and critical thinking abilities required for successful careers in academia, industry, or research.

The MSc Chemistry program consists of a comprehensive curriculum that includes a combination of core courses, elective courses, laboratory work, Industrial/Institutional visits, internships, and a research project. The program allows students to specialize in specific areas of chemistry based on their interests and career aspirations. The course consists of four theory papers each and three practical papers in the 1<sup>st</sup> and II<sup>nd</sup> semesters. There will be three theory papers, one open/multi-disciplinary elective paper, and three practical papers (to be continued in semester IV) in the III<sup>rd</sup> semester. Two elective papers, three practical papers, a project, an industrial/institutional visit/ internship along with a general viva voce will be there in the IV<sup>th</sup> semester. The students may select one elective paper from each of the elective groups. Each theory paper and elective paper is of 3 hours duration and each practical paper is of 6 hours duration. The total marks for the entire course shall be 1500 and the total credit shall be 80. 20% of marks shall be allocated for internal assessment of theory and practical papers each. The PG programme shall extend over a period of two academic years comprising four semesters, each of 450 hours in 18 weeks duration.

The program utilizes continuous assessment methods to measure and evaluate student learning outcomes. These assessments may include examinations, laboratory reports, research papers, presentations, and project work. Feedback and constructive criticism are provided to facilitate student growth and improvement.

Graduates of the MSc Chemistry program will be well-prepared for diverse career paths. They can pursue employment opportunities in research and development laboratories, pharmaceutical and chemical industries, government agencies, educational institutions, and more. The program

also lays a strong foundation for those interested in pursuing further studies and research at the doctoral level.

The MSc Chemistry program, aligned with Outcome-Based Education, offers students a comprehensive education in chemistry and prepares them for successful careers in the field. By focusing on defined outcomes and emphasizing practical skills, critical thinking, and research abilities, the program ensures that students are well-equipped to address the challenges and contribute to advancements in the field of chemistry.

#### 2. VISION AND MISSION STATEMENTS

#### Vision:

To establish a teaching, residential, and affiliating University and to provide equitable and just access to quality higher education involving the generation, dissemination, and critical application of knowledge with a special focus on the development of higher education in Kasaragod and Kannur Revenue Districts and the Manantavady Taluk of Wayanad Revenue District.

#### Mission:

> To produce and disseminate new knowledge and to find novel avenues for the application of such knowledge.

> To adopt critical pedagogic practices which uphold scientific temper, the uncompromised spirit of inquiry, and the right to dissent.

 $\succ$  To uphold democratic, multicultural, secular, environmental, and gender-sensitive values as the foundational principles of higher education and to cater to the modern notions of equity, social justice, and merit in all educational endeavours.

To affiliate colleges and other institutions of higher learning and to monitor academic, ethical, administrative, and infrastructural standards in such institutions.

➤ To build stronger community networks based on the values and principles of higher education and to ensure the region's intellectual integration with national vision and international standards.

➤ To associate with the local self-governing bodies and other statutory as well as nongovernmental organizations for continuing education and also for building public awareness on important social, cultural, and other policy issues.

#### **3. THE PROGRAMME OUTCOMES (POs)**

Programme Outcomes (POs): Programme outcomes can be defined as the objectives achieved at the end of any specialization or discipline. These attributes are mapped while a student is doing graduation and determined when they get a degree.

PO 1. Advanced Knowledge and Skills: Postgraduate courses aim to provide students with in-depth knowledge and advanced skills related to their chosen field. The best outcome would be to acquire a comprehensive understanding of the subject matter and develop specialized expertise.

PO 2. Research and Analytical Abilities: Postgraduate programs often emphasize research and analytical thinking. The ability to conduct independent research, analyze complex problems, and propose innovative solutions is highly valued.

PO 3. Critical Thinking and Problem-Solving Skills: Developing critical thinking skills is crucial for postgraduate students. Being able to evaluate information critically, identify patterns, and solve problems creatively are important outcomes of these programs.

PO 4. Effective Communication Skills: Strong communication skills, both written and verbal, are essential in various professional settings. Postgraduate programs should focus on enhancing communication abilities to effectively convey ideas, present research findings, and engage in academic discussions.

PO 5. Ethical and Professional Standards: Graduates should uphold ethical and professional standards relevant to their field. Understanding and adhering to professional ethics and practices are important outcomes of postgraduate education.

PO 6. Career Readiness: Postgraduate programs should equip students with the necessary skills and knowledge to succeed in their chosen careers. This includes practical skills, industry-specific knowledge, and an understanding of the job market and its requirements.

PO 7. Networking and Collaboration: Building a professional network and collaborating with peers and experts in the field are valuable outcomes. These connections can lead to opportunities for research collaborations, internships, and employment prospects.

PO 8. Lifelong Learning: Postgraduate education should instill a passion for lifelong learning. The ability to adapt to new developments in the field, pursue further education, and stay updated with emerging trends is a desirable outcome.

#### 4. PROGRAMME SPECIFIC OUTCOMES OF MSc CHEMISTRY

Program Specific Outcomes (PSOs) serve as a framework to outline the specific goals and expected learning outcomes of the MSc Chemistry program. These outcomes are designed to ensure that graduates possess the necessary knowledge, skills, and abilities to excel in their careers or pursue further research in the field of chemistry. The Programme Specific Outcomes are given below.

PSO 1. In-depth knowledge of core concepts: Understanding of the fundamental principles and theories in various sub-disciplines of chemistry, including organic, inorganic, physical, analytical, and theoretical chemistry.

PSO 2. Advanced laboratory skills: Possess advanced laboratory skills necessary for planning, executing, and analyzing experiments in diverse areas of chemistry. This includes skill in handling chemical reagents, instruments, and equipment, as well as accurate measurement techniques.

PSO 3. Research and scientific inquiry: Exhibit competence in designing and conducting independent research projects in chemistry, including formulating research questions, implementing methodologies, collecting and interpreting data, and drawing appropriate conclusions.

PSO 4. Critical thinking, data analysis, interpretation, and problem-solving: Apply critical thinking skills to analyze complex chemical problems and propose innovative solutions. Effective in interpreting experimental data using appropriate statistical methods and computational tools.

PSO 5. Effective communication: Communicate scientific ideas, research findings, and complex concepts effectively through written reports, research papers, and oral presentations. PSO 6. Safety and ethical practices: Awareness of ethical principles and safety protocols in all aspects of chemical research and laboratory work.

PSO 7. Interdisciplinary knowledge and collaboration: Display the ability to integrate knowledge from various fields, collaborate with interdisciplinary teams, and apply chemical principles to solve problems in related areas, such as environmental science, materials science, pharmaceuticals, biochemistry, nanoscience, etc.

#### **5. THE COURSE OUTCOMES**

Course Outcomes (COs): Course outcomes are the objectives that are achieved at the end of any semester/year. For instance, if a student is studying a particular course, then, the outcomes would be concluded on the basis of the marks or grades achieved in theory and practical lessons.

The COs are set at the beginning of the study of each course.

# 6. THE COURSE STRUCTURE, SCHEME & CREDITS

6.1 The course structure, syllabus, and scheme are given below.

Semester	Paper Code	Title	Hrs /wk	Exam Durati on	Marks for ESA	Mark s for CA	Total	Credit
	MSCHE01C01	Theoretical Chemistry - I	4	3	60	15	75	4
	MSCHE01C02	Inorganic Chemistry - I	4	3	60	15	75	4
	MSCHE01C03	Organic Chemistry - I	4	3	60	15	75	4
1	MSCHE01C04	Physical Chemistry - I	4	3	60	15	75	4
	MSCHE01C05	Inorganic Chemistry Practical - I	3	Carried	over to	seme	ster - I	1
	MSCHE01C06	Organic Chemistry Practical - I	3	Carried	d over to	semes	ster - I	1
	MSCHE01C07	Physical Chemistry Practical - I	3	Carried	d over to	o semes	ster - I	I
		Total :	25		240	60	300	16
	MSCHE02C08	Theoretical Chemistry - II	4	3	60	15	75	4
	MSCHE02C09	Inorganic Chemistry - II	4	3	60	15	75	4
	MSCHE02C10	Organic Chemistry - II	4	3	60	15	75	4
11	MSCHE02C11	Physical Chemistry - II	4	3	60	15	75	4
	MSCHE01&02C05	Inorganic Chemistry Practical - I	3	6	40	10	50	2
	MSCHE01&02C06	Organic Chemistry Practical - I	3	6	40	10	50	2
	MSCHE01&02C07	CHE01&02C07 Physical Chemistry Practical - I				10	50	2
	Total :				360	90	450	22
	MSCHE02001	Open Elective Paper I*	1	3	60	15	75	4
	MSCHEUSOU1	(Multidisciplinary)	4	5	00	10	10	
	MSCHE03C12	Inorganic Chemistry - III	4	3	60	15	75	4
	MSCHE03C13	Organic Chemistry - III	4	3	60	15	75	4
	MSCHE03C14	Physical Chemistry - III	4	3	60	15	75	4
1	MSCHE03C15	Inorganic Chemistry Practical - II	3	Carried	d over to	o seme	ster -	V
	MSCHE03C16	Organic Chemistry Practical - II	3	Carrie	d over to	o seme	ster -	V
	MSCHE03C17	Physical Chemistry Practical - II	3	Carrie	d over to	o seme	ster -	V
	MSCHE03C18	Industrial Visit/Institutional Visit/Internship		Carrie	Carried over to semester - IV			IV
		Total :	25		240	60	300	16
	MSCHE04E01	Elective Paper II*	4	3	60	15	75	4
	MSCHE04E02	Elective Paper III*	4	3	60	15	75	4
	MSCHE03&04C15	Inorganic Chemistry Practical - II	3	6	40	10	50	2
	MSCHE03&04C16	Organic Chemistry Practical - II	3	6	40	10	50	2
IV	MSCHE03&04C17	Physical Chemistry Practical - II	3	6	40	10	50	2
	MSCHE03&04C18	Industrial Visit/Institutional Visit/Internship			30	5	35	2
	MSCHE04C19	Project (With Presentation)	8		60	15	75	6
	MSCHE04C20	Viva Voce (General)			40		40	4
	the second second	Total :	25	The second	370	80	450	26

# COURSE STRUCTURE

S	Semesterwise Split-up of Marks									
Se m	Hrs allott ed	Marks for ESA	Mark s for CA	Total Marks	Credit					
Ι	25	240	60	300	16					
	25	360	90	450	22					
	III 25 240			300	16					
IV	25	370	80	450	26					
	100	1210	290	1500	80					

6.2 The semester-wise split-up of marks is given below.

**6.3 Elective Papers:** The students may choose one open elective (multidisciplinary) from the following set 1 for semester III, and two elective papers for semester IV from groups II and III.

	ELECTIVE PAPERS							
Sem	Elective No	Paper Code	Title					
	The State State of State	MSCHE03O01	Food Chemistry					
III	I (Open Elective/ Multidisciplinary	MSCHE03O02	Environmental Chemistry and Disaster Management					
		MSCHE03O03	Medicinal Chemistry					
IV	II	MSCHE04E01	Interdisciplinary topics and instrumentation techniques					
IV		MSCHE04E02	Computational Chemistry					
		MSCHE04E03	Biochemistry					
		MSCHE04E04	Nanomaterial Chemistry					
IV	III	MSCHE04E05	Polymer Chemistry					
		MSCHE04E06	Material Chemistry					

#### 6.4 Project Work and Viva Voce

a) Each student shall carry out project work in one of the broad areas of theoretical/Organic/physical/environmental/inorganic chemistry for a period of a minimum of 12 weeks duration in the IV<sup>th</sup> semester under the supervision of a teacher of the department. A student may, in certain cases be permitted to do the project work in an industrial/research organization on the recommendation of the department coordinator. In such cases, one of the teachers from the department shall act as co-supervisor.

b) The candidate shall submit 2 copies of the dissertation based on the results of the project work at the end of the program.

c) Every student has to do the project work independently. No group projects are accepted. The project should be unique with respect to the title, project content, and project layout. No two project reports of any students should be identical, in any case as this may lead to the cancellation of the project report by the university.

d) The ESE of the project work shall be conducted by two external examiners. The evaluation of the project will be done in two stages.

i. Internal evaluation (supervising teacher/s will assess the project and award internal marks)

ii. External evaluation (by external examiners appointed by the university)

e) Pass conditions

i. The student shall declare to pass the project report course if she/he secures a minimum of 40% marks (internal and external put together). In an instance of the inability of obtaining a minimum of 40% marks, project work may be redone and the report may be resubmitted along with subsequent exams through the parent department. There shall be no improvement chance for the marks obtained in the project report.

f) Assessment of different components of the project may be taken as below

Internal (Viva) 20% of total		External (80% of Total)				
Components	% of internal Components marks		% of external marks			
Punctuality	10	Relevance of topic and Structure of Report	20			
Use of data	10	Quality of Analysis/ use of statistical tools	20			
Scheme Organization of	30	Findings and recommendations	20			
Viva-voce	50	Presentation of Project Report	20			
		Viva-voce	20			

PROJECT

g) Viva-voce shall be conducted by two examiners; both of them shall be external examiners. Viva-voce is based on theory and practical papers of all semesters including elective papers

#### 6.5 Internship/ Industrial Visit/ Institutional Visit

a) Internships provide hands-on experience in real-world chemistry settings, allowing postgraduates to apply their theoretical knowledge in practical scenarios. This experience enhances their understanding of laboratory techniques, equipment, and experimental procedures. Each student shall undergo an internship for a period of a minimum of two weeks duration or visit a minimum of two or more institutions/ industries of national/international importance in any of the I<sup>st</sup> to IV<sup>th</sup> semesters and the report should be submitted during IV<sup>th</sup> semester practical examination along with project evaluation / Viva voce.

b) The candidate shall submit a copy of the IV/internship report during the IV<sup>th</sup> semester project evaluation / Viva voce.

#### 6.6 Continuous assessment

a) This assessment shall be based on a predetermined transparent system involving periodic written tests, assignments, and seminars in respect of theory courses and based on tests, lab skills, records, and viva in respect of practical courses.

b) The percentage of marks assigned to various components for internal is as follows

	Theory							
No	Components	% of internal marks						
1	Two test paper	50						
2	Assignments	25						
3	Seminars/Presenta tion of case study	25						

	Practicals							
No	Components	% of internal marks						
1	Two test paper	40						
2	Lab skill	20						
3	Record	20						
4	Viva	20						

#### 6.7 Grading system

The seven-point indirect grading system is followed and the guidelines for grading are as follows

SI N 0	% of Marks	Grade	Interpretation	Range of Grade Points	Class
1	90 and above	A+	Outstanding	9.0 - 10	First class with
2	80 to below 9	A	Excellent	8.0 - 8.9	distinction
3	70 to below 8	В	Very Good	7.0 - 7.9	First class
4	60 to below 7	С	Good	6.0 - 6.9	First class
5	50 to below 6	D	Satisfactory	5.0 - 5.9	Second Class
6	40 to below 5	E	Pass/Adequate	4.0 - 4.9	Pass
7	Below 40	F	Failed	0.0 - 3.9	Fail

#### **GRADING PATTERN**

# 6.8 Guidelines for the preparation of a dissertation on the project:

6.8.1. Arrangement of contents shall be as follows:

- 1. Cover page and title page
- 2. Bonafide certificate
- 3. Declaration by the student
- 4. Acknowledgement
- 5. Table of contents
- 6. List of tables

7. List of Figures

8. List of symbols, Abbreviations and Nomenclature

9. Chapters

- 10. Appendices
- 11. References

#### 6.8.2. Page dimension and typing instructions:

The dimension of the dissertation on the project should be in A4 size. The dissertation should be typed on bond paper and bound using a flexible cover of thick white art paper or spiral binding. The general text shall be typed in the font style 'Times New Roman' and font size 12. For major headings font size may be 16 and minor heading 14. Paragraphs should be arranged in justified with a margin of 1.25 each on top. Portrait orientation shall be there on the left and right of the page. The content of the report shall be around 40 pages.

#### 6.8.3. Bonafide certificate shall be in the following format

#### CERTIFICATE

Office seal Date

Signature, name, designation, and official address of the Supervisor.

#### 6.8.4. Declaration by the student shall be in the following format:

#### DECLARATION

Date:

Signature and name of the student

# 7. PATTERN OF QUESTION PAPERS

The pattern of question papers, time, and difficulty level for theory papers will be as follows

Section	Criteria	Time	Marks				Percentage	Revised Taxonomy/Level	
А	5 out of 6 questions (short answer questions)	5 x 8 min = 40 min	5	×	3	=	15	25	1,2 (Remember, Understand)
В	3 out of 5 questions (paragraph questions)	3 x 20 min = 60 min	3	×	6	=	18	30	5, 6 (Evaluate, Create)
С	3 out of 5 questions (essay-type questions)	3 x 25 min = 75 min	3	×	9	=	27	45	3, 4 (Apply, Analyze)
	Total =					60	100	100	

The distribution of questions will be as follows

Distribution of Questions										
Units	Units Unit 1 Unit 2 Unit 3 Unit 4									
Number of Questions	4	4	4	4						

#### **SEMESTER-1**

#### **MSCHE01C01: THEORETICAL CHEMISTRY - I**

#### Credit: 4

#### TIME: 72 HOURS

#### Course Outcomes: After the completion of the course, the learners should be able to

- CO 1. Understand and examine the basic principles of Quantum Mechanics
- CO 2. Apply the postulates of quantum mechanics to simple systems
- CO 3. Make use of the approximation methods to calculate the properties of simple systems
- CO 4. Demonstrate the principles of chemical bonding in diatomic and polyatomic molecules
- CO 5. Apply HMO theory to simple conjugated systems

#### **UNIT -1: QUANTUM MECHANICS-I**

#### **18 Hours**

Historical development of Quantum Mechanics- Max Plank's Quantum Theory of Radiation - Photoelectric effect- Black body radiation – Compton effect – Wave-particle duality of matterde-Broglie concept – Electron diffraction – Davison and Germer Experiment – Electron double slit experiment- Stern- Gerlach Experiment- Heisenberg's uncertainty Principle. Complex Numbers – definition - complex conjugate absolute values of a complex number – complex functions. Schrödinger wave mechanics – Deduction of Schrodinger equation from classical wave equation. The physical meaning of wave function. Normalized and orthogonal function. Elements of operator algebra: definition – linear non–linear operators – commuting and non-commuting operators-vector operators – Laplacian operators and their expressions in spherical polar coordinates (derivation not required). Eigenfunctions and Eigenvalues– Hermitian operators. Formulation of quantum mechanics: The postulates of quantum mechanics – state function postulate – operator postulate – Eigen value postulate – Expectation value postulate – Postulate of time-dependent Schrödinger equation stationary states and time-independent Schrödinger equation.

#### UNIT - II: QUANTUM MECHANICS - II

#### **18 Hours**

Translational motion: Particle in a one-dimensional box-complete treatment – particle in a threedimensional box (rectangular and cubical box) – degeneracy.

Quantum mechanics of vibrational motion One-dimension Harmonic oscillator – complete treatment – Hermite polynomials – Recursion formula- comparison of classical and quantum mechanical results.

Quantum Mechanics of rotational motion: Particle on a ring (Planar rigid rotator)- Particle on a sphere (Nonplanar rigid rotator) – the wave function in spherical polar co-ordinates – complete treatment – Legendre polynomial –Rodrigue's formula- spherical harmonies –wave function in the real form- polar diagrams-

Quantum mechanics of Hydrogen like atoms: potential energy of hydrogen-like atoms – the wave equation in spherical polar co-ordinates – solution of the R,  $\theta$ ,  $\phi$  equations – Laguerre polynomials – associated Laguerre polynomials – Discussion of the wave functions –radial function, radical distribution function and angular function and their plots– orbitals and orbital diagrams – their significance.

#### **UNIT - III: QUANTUM MECHANICS - III**

#### **18 Hours**

**18 Hours** 

Need of approximate methods in quantum chemistry: variation method – variation theorem with proof –illustration of variation theorem using a trial function [e.g., x (a-x)] for the particle in a 1D-box and using the trial function  $e - \Box r^2$  for the hydrogen atom, variation treatment for the ground state of helium atom;

Perturbation method: time-independent first-order correction to the energy and wave function, second-order correction to energy– illustration by application to particle in an ID-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Electron spin and atomic structure: spin functions and operators –spin-orbit interactions – Angular momentum – commutation relations – operators Term symbols – Russel – Saunder's terms and coupling schemes – introduction to SCF methods – Hartree and Hartree – Fock's SCF.

#### **UNIT - IV: CHEMICAL BONDING**

# Born – Oppenheimer approximation – essential principles of the MO method – MO treatment of Hydrogen molecule and the $H_2$ + ion – valence bond treatment of the ground state of hydrogen molecule – MO treatment of homonuclear diatomic molecules (quantitative) – Li<sub>2</sub>, Be<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, O<sub>2</sub>+, O<sub>2</sub>-, F<sub>2</sub> and heteronuclear diatomic – LiH, CO, NO, HF – theory of chemical bonding for polyatomic molecules – Abinitio calculations – basic principles — basis sets – STO and GTO – Spectroscopic term symbols for diatomic molecules.

Localized bonds – hybridization and geometry of molecules – methane, ethene, acetylene (bond angle, dihedral angle, bond length, and bond energy) – HMO theory of ethylene, butadiene, and benzene - aromaticity- bond order, charge density, and free valence calculations

#### REFERENCE

1. N Levine, Quantum Chemistry 5th Ed. Prentice Hall India

2. R. Anantharaman, Fundamentals of Quantum Chemistry, Mc Millan India

3. A. K. Chandra, Introductory Quantum Chemistry - 4th Ed. Tata Mc Graw Hill

4. D. A. McQuarrie Quantum Chemistry, University Science Books

5. L. Pauling and W.B Wilson, Introduction to Quantum Mechanics, McGraw Hill

6. R. K. Prasad, Quantum Chemistry 4th Ed. New Age International

7. P. W. Atkins, Molecular Quantum Mechanics, Oxford University Press

8. M.S.Day and J.Selbin, Theoretical Inorganic Chemistry, East West Books

 Tamas Veszpremi and Miklos Feber, "Quantum Chemistry – Fundamentals to Applications" Springer.

9. Quinn – "Computational Quantum Chemistry – An Interactive Guide to Basis Set theory"- Ane Books Pvt. Ltd.

10. Thomas Engel- Quantum Chemistry and Spectroscopy, 4th Edition, Pearson

#### **MSCHE01C02: INORGANIC CHEMISTRY - I**

#### Credit: 4

#### **TIME: 72 HOURS**

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1: Apply the theory of precipitation phenomena in the determination of metal ions

CO 2: Impart advanced knowledge of the theory of complexometric titration

CO 3: Predict the stabilities of complexes based on the HSAB principle

CO 4: Understand different types of Non- aqueous solvents and their applications

CO 5: Develop and attain advanced knowledge of nuclear Chemistry and radiation Chemistry and their applications

CO 6: Demonstrate the preparation, structure, and properties of compounds of Boron, Phosphorous, and Nitrogen

#### **UNIT - I: THEORETICAL BASIS OF ANALYSIS**

Precipitation phenomena – precipitation from homogenous solution, organic precipitants in inorganic analysis (Dimethyl glyoxime, cupferron, oxine reagent, cupron, nitron, anthranilic acid) – extraction of metal ions – nature of extractants – distribution law – partition coefficients – types of extraction and applications

Analytical applications of complex formation; Gravimetric analysis - Ni, Cu, - Chelometric titrations (a detailed study) – titration curves with EDTA – feasibility of EDTA titration – indicators for EDTA titration and its theory (a detailed study) – selective masking and demasking techniques – industrial application of masking

Automated Techniques - Flow injection Analysis - Method and Instrumentation

Electrogravimetry - Theory, apparatus, and application- Determination of copper.

#### UNIT-II ACIDS, BASES, AND NON-AQUEOUS SOLVENTS

A generalized acid-base concept - Measure of acid-base strengths – gas phase basicities – proton affinities – gas phase acidities – proton loss gas phase acidities – electron affinities – systematic of Lewis acid-base interaction – bond energies – steric effect – proton sponges. Solvation effects and acid-base anomalies. Hard and soft acids and bases – classification – strength and hardness and softness – symbiosis – theoretical basis of hardness and softness – electron negativity and hardness and softness.

#### **18 Hours**

**18 Hours** 

Superacids and bases - Types, examples, and applications

Classification of solvents – properties of nonaqueous solvents like HF,  $N_2O_4$ , and  $SO_2$  – chemistry of molten salts as nonaqueous solvent systems – solvent properties – room temperature molten salts – nonreactivity of molten salts - solution of metals –

Ionic liquids as green solvents, room temperature ionic liquids, and supercritical fluids. Use of nonaqueous solvents in synthesis

#### **UNIT – III NUCLEAR AND RADIATION CHEMISTRY**

Nuclear models – shell, liquid drop, Fermi gas, Collective and optical models – Assumptions, merits, and demerits– equation of radioactive decay – half-life and average life. Radioactive equilibrium – transient and secular equilibrium – Bethe's notation for nuclear processes - types of nuclear reaction – neutron capture cross section and critical size – principles and working of GM and scintillation

**18 Hours** 

counters.

Basic principles of nuclear reactors - types of reactors - PHWR, BWR

Elements of radiation chemistry – introduction- the interaction of ionizing radiation with matter. LET for charged particle due to collision with electron. Bremsstrahlung interaction of electromagnetic radiation with matter. Radiolysis of water - Radiation dosimetry - Fricke Dosimeter- Applications of radiation chemistry – Rock dating, Nuclear Activation Analysis, Tracer techniques, Medicine, Industry

# UNIT-IV BORON, PHOSPHORUS, AND NITROGEN COMPOUNDS 18 Hours

The neutral boron hydrides – structure and bonding topological approach to boron hydride structure – Styx number – synthesis and reactivity of neutral boron hydrides. Importance of icosahedral framework of boron atoms in boron chemistry – closo, nido, and arachno structure – Wades rule – mno rules

Carboranes–Structure and classification - preparation and properties of dicarba- closododecaboranes  $(C_2B_{10}H_{12}$  - ortho, meta, and para) - metallocarboranes – preparation and structure of metallo carboranes of Fe & Co

Phosphorous sulphides  $-P_4S_3$ ,  $P_4S_5$ ,  $P_4S_7$ , and  $P_4S_{10}$  – preparation, properties, structure, and uses. The phosphazenes (phosphonitrilic halides)

Sulphur nitrogen compounds –  $S_2N_2$  and  $S_4N_4$  – Polythiazyl, other  $S_XN_Y$  compounds. Their preparation properties, and structure.

Poly acids - Iso poly and heteropoly acids of Mo & W elements - Structure and formation

#### REFERENCES

- F A Cotton, Wilkinson, C A Murrillo and M Bochmann "Advanced Inorganic Chemistry 6<sup>th</sup> edition, John Wiley and Sons Inc
- 2) Vogel's Textbook of Quantitative Chemical Analysis Fifth Edition
- Bodie Douglas, Darl H Mc Daniel and John J Alexander, Concepts and models of Inorganic Chemistry, John Wiley and Sons Inc 3<sup>rd</sup> edition
- 4) G N Jeffery, J Basette, J Mendham and R C Denny, Vogel's textbook of quantitative chemical analysis (Vth edition), John Wiley and Sons
- 5) H Sisler, Chemistry of non-aqueous solvents, Reinhold
- J E Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Person Education India
- 7) G Friedlander and J W Kennedy, Introduction to radiochemistry, John Wiley and Son Inc
- 8) S Glasston, a Sourcebook on atomic energy, Van Nostrand
- H J Arniker, Essentials of Nuclear Chemistry, New age international, New Delhi 4<sup>th</sup> edition 1995
- 10) J D Lee, Concise Inorganic Chemistry (IVth edition) Oxford University Press
- S K Agarwal and Keemti Lal, Advanced Inorganic Chemistry, Pragati Prakashan 9<sup>th</sup> Edition 2009
- 12) B K Sharma, Instrumental Methods of Chemical Analysis, Goel publishing house, 2000
- 13) Duward F Shriver, Peter William, Atkins, Cooper Harold Langford, Inorganic Chemistry
- 14) M G Arora and M Singh, Nuclear chemistry
- 15) Walter D Loveland, David J Morrissey, Glenn T Seaborg, Modern Nuclear Chemistry
- 16) Catherine E Housecroft and Alan G Sharpe. Inorganic Chemistry, 4th Edition, Pearson
- 17) George A Olah, G K Surya Prakash Superacid Chemistry, 2nd Edition, Wiley

#### Credit: 4

#### **TIME: 72 HOURS**

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Study the various reaction intermediates in organic reactions.

CO 2. Investigate the role of reaction conditions and reagents in the generation of intermediates.

CO 3. Formulate a mechanism for the suggested reactions.

CO 4. Analyze the structure-property relations in aliphatic substitution reactions. Apply the concept of elimination to various organic molecules.

CO 5. Understand the various aromatic systems and their reactions. Classify molecules based on the aromatic behavior.

CO 6. Study the different photochemical reactions and apply to natural photochemical reactions.

#### **UNIT- I: Reaction intermediates and Rearrangements**

#### (18 Hours)

(18 hours)

Structure, formation, and properties of carbenes, nitrenes, and arynes – singlet and triplet carbenes, nitrenes and arynes, Carbon free radicals: structure, formation, and stability. Structure, stability, and formation of Ylides, Enamines, 1,3-dithiane, Benzynes, and Enolates.

Molecular rearrangement mechanism. Carbon to carbon migration: Wagner Meerwein, Pinacol, Wolff, Benzilic acid, Demjanove, Dienone-phenol, Hoffmann-Martius. Carbon to nitrogen migration: Hofmann, Curtius, Schmidt, Lossen, Beckmann. Migration to electron-rich carbon: Wittig, Wittig-Hormer, Favorski, Stevens, Neber Orton, Bamberger. Migration to electron-deficient oxygen: Baeyer, villager, Darkin reaction. Aromatic rearrangements: benzidine, Fries, Von-Richter Sommlet-Hauser,

# **UNIT-2: Substitution and Elimination Reactions**

Aliphatic nucleophilic substitution reactions – saturated and unsaturated systems – Mechanism of nucleophilic substitution – SN2, SN1, SNi, SET. Neighbouring group participation – non-classical carbocations. Substitution at allylic and vinylic carbon atoms. Effect of substrate structure, attacking nucleophile, leaving group, and reaction medium on reactivity and regioselectivity. Aliphatic Electrophilic substitutions: SE1 SE2 and SEi mechanisms with suitable examples.

Elimination Reaction: Mechanistic and stereochemical aspects of E1, E2, and E1cB eliminations. The

effect of substrate structure, base, leaving group, and reaction medium on elimination reactions. Elimination reaction in 4-t-Butylcyclohexyl tosylate (cis and trans), 2- Phenylcyclohexanol (cis and trans), Menthyl and neomenthyl chlorides, and benzene hexachlorides. Saytzev vs Hofmann elimination, Bredt's rule,  $\alpha$ - elimination, pyrolytic syn elimination (Ei) – Chugaev reaction, and Cope elimination. Dehydration of alcohols, Dehalogenation of vicinal dihalides, and Peterson elimination.

#### **UNIT-3: Aromaticity and Aromatic Reactions**

#### (18 Hours)

MO description of aromaticity and antiaromaticity. Homoaromaticity. Aromaticity of annulenes and heteroannulenes, fused ring systems, fulvenes, fulvalenes, azulenes, pentalenes, and heptalenes. mesoionic compounds, metallocenes, cyclic carbocations, and carbanions. Effect of delocalized electrons on pKa.

Aromatic Electrophilic Substitution: Arenium ion mechanism, substituent effect on reactivity in mono and disubstituted benzene rings, *ortho/para* ratio, *Ipso* substitution. Relationship between reactivity and selectivity.

Aromatic Nucleophilic substitution: Addition-elimination (SNAr) mechanism, elimination-addition (benzyne) mechanism, *cine* substitution, SN1 and SRN1 mechanism. The effect of substrate structure, nucleophile, and leaving group on aromatic nucleophilic substitution. Nucleophilic Substitution of Pyridine-Chichibabin Reaction.

#### **UNIT-4: Photochemistry**

#### (18 Hours)

Photochemical excitation of molecules, spin multiplicity, Jablonski diagram, photosensitization, and quenching. Photochemistry of carbonyl compounds: Norrish type- I cleavage of acyclic, cyclic, and  $\beta$ ,  $\gamma$ - unsaturated carbonyl compounds. Norrish type- II cleavage, photo reduction, photoenolization. Photocyclo- addition of ketones with unsaturated compounds: Paterno- Büchi reaction, photodimerization of  $\alpha$ ,  $\beta$ - unsaturated ketones, Photo rearrangements: Photo –Fries, di-  $\pi$ - methane, oxa di-  $\pi$ - methane, aza di-  $\pi$ - methane, lumi ketone rearrangements. Barton and Hoffmann- Loeffler-Freytag reactions. Photo isomerization and dimerization of alkenes, photo isomerization of benzene and substituted benzenes, and photo-oxidation. Photochemistry of vision and photosynthesis.

#### **References:**

1. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.

2. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5/e., Springer, 2007.

3. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford

University Press, 2004.

4. R.O.C.Norman & J.M.Coxon, Principles of Organic Synthesis, 3/e, Nelson Thornes

5. J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6/e, Wiley, 2007.

6. Ahluwalia Mukherjee and Singh, Organic reaction mechanisms

7. Maya Shankar Singh, Advanced organic chemistry: reactions and mechanisms, Pearson

8. Peter Sykes, A guidebook to mechanism in organic chemistry, 6th eed Pearson

9. I L Finar, Organic Chemistry Volume 2, Pearson Education.

10. P.S. Kalsi, Organic reactions & their mechanisms, 3/e revised, New Age International Publishers.

11. Modern methods of organic synthesis, Carruthers,

12. P.S.Kalsi, Organic reactions & their mechanisms, 3/e revised, New Age International Publishers.

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

#### **MSCHE01C04: PHYSICAL CHEMISTRY - I**

#### Credit: 4

#### **TIME: 72 HOURS**

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Illustrate the concepts of the third law of thermodynamics and thermodynamic irreversibility.

CO 2. Analyze phase transitions and phase diagrams of three component systems.

CO 3. Develop an understanding of the theoretical aspects of electrochemical activities and various facets of electrochemistry.

CO 4. Interpret the mechanism of electrode-electrolyte interaction.

CO 5. Analyze different aspects of the electrode process.

CO 6. Illustrate the importance and concepts of electrochemistry in other fields like supercapacitors, batteries, and corrosion.

#### UNIT-1: THERMODYNAMICS AND PHASE EQUILIBRIA 18 Hours

**Thermodynamics**: Third law of thermodynamics- need for third law, Nernst heat theorem, determination of absolute entropies using third law, Residual entropy. entropy changes in chemical reactions. Thermodynamic equations of state.

Partial molar quantities - chemical potential-variation of chemical potential with T&P- determination of partial molar volume and enthalpy. Thermodynamic functions of ideal gases, real gases, and gas mixtures- Entropy and free energy of mixing. Excess thermodynamic functions. Thermodynamics of irreversible processes with simple examples. The general theory of nonequilibrium processes. Entropy production. The phenomenological relations. Principle of microscopic reversibility, Onsager reciprocal relations. Application to the theory of diffusion, thermo-osmosis, and Thermoelectricity (Seebeck effect, Peltier effect, and Thomson effect).

**Phase equilibria:** Phase rule -Physical equilibria involving phase transition-criteria for equilibrium between phase-Three component system- graphical representations-solid liquid equilibria Ternary solution with common ion-Hydrate formation-compound formation-liquid-liquid equilibria-one pair of partially miscible liquids-two pairs of partially miscible liquids-three pairs of partially miscible liquids.

#### **UNIT-2: ELECTROCHEMISTRY**

The nature of electrolytes– Ionic mobilities- ion activity- ion-ion and ion -solvent interaction. Equilibrium properties of electrolyte solutions. Electrolytes of the first and second kind, - Influence of pressure and temperature on ion conductance-Walden's equation- Abnormal ion conductance-Derivation of Debye-Huckel Onsager equation- the validity of Debye-Huckel-Onsager equation for aqueous and non-aqueous solution-Deviation from Onsager equation-Conductance ratio and Onsager equation-Dispersion of conductance at high frequencies-Triple ion conductance minima-Equilibria in electrolytes-Association constant Ion-association-dissociation constant--- Activities and activity coefficient in electrolytic solutions.-Debye-Huckel limiting law and its various form, qualitative and quantitative tests of Debye-Huckel limiting equation. Osmotic coefficient- solubility product principle-solubility in the presence of common ion-Activity coefficient and solubility measurement.

#### **UNIT-3: ELECTRODICS**

# Liquid junction potential. The electrode double layer-electrode-electrolyte interface-Theory of multilayer capacity. Electric capillary Lippmann -potential, Membrane-potential. Butler Volmer equation for simple electron transfer reaction-Transfer coefficient- Exchange current density Rate constants- Tafel equation and its significance.

Electrolytic polarization- dissolution and deposition potentials, concentration polarization. Decomposition voltage and its determination.

Overvoltage - hydrogen and oxygen overvoltage, metal deposition over-voltage, and their determination. Theories of overvoltage.

Cyclic Voltammetry- Theory and experimental setup, Cyclic voltammogram.

Polarography- Principle and instrumentation Dropping mercury electrode- half-wave potential and Ilkovic equation

# UNIT-4: APPLIED ELECTROCHEMISTRY AND CORROSION 18 Hours

**Energy storage devices**: Batteries- Working of Lithium-ion battery. Basics of supercapacitors, Classification with examples. Electrostatic double layer capacitors (EDLC) and Psuedo capacitors-working and principle.

**Corrosion**: Thermodynamics of corrosion and electrode potentials. EMF of a cell-measurement- emf calculation of half cell potential-Nernst equation. Basis of Pourbaix diagrams- Diagrams of water, Fe, and Al. Limitations of Pourbaix diagrams. Kinetics of corrosion- Polarization and corrosion rate. Measurement of polarization- causes of polarization. Calculation of

#### **18 Hours**

**18 Hours** 

IR drops in an electrolyte. Influence of polarization on corrosion rate. Polarization diagram of corroding metals. Calculation of corrosion rate from polarization data. Theory of cathode protection. Passivity.

#### REFERENCES

- 1. Rastogi and Misra-"An Introduction to chemical thermodynamics-6thedition"- Vikas publishing.
- 2. S. Glasstone-"Thermodynamics for chemists"-Affiliated East West publication.
- 3. Lewis and Randal-"Thermodynamics"-McGraw-Hill.
- 4. Daniels and Alberty-"Physical Chemistry"- John Wiley.
- 5. "Mathematics of physics and chemistry"- Murphy, George M., Margenau, Henry
- 6. S. Glasstone-"Theoretical electrochemistry"-East-West Books
- 7. L.I.Anthropov-"Theoretical electrochemistry"-Mir publishers.
- 8. Bockris and Reddy-"Modern electrochemistry"-Springer
- 9. G.W. Castellan "Physical chemistry"- Narosa
- 10. I. Pregogine-"Introduction of Irreversible to thermodynamics process"-Interscience
- 11. G.M. Barrow- Physical Chemistry- Tata McGraw-Hill.
- 12. Duta K. Robin "Physical Chemistry" AbeBooks
- 13. Winston Revie and Herbert Uhlig, Corrosion and corrosion control:(Wiley) Edited by L. L.
- Shreir, G. T. Burstein, R. A. Jarman Corrosion ControlVolume2:
- 14. Fontana and Greene Corrosion Engineering:
- 15. What are batteries, fuel cells, and supercapacitors? Chem Rev. 2004, 104, 4245-4269
- 16. Electrochemical methods: Fundamentals and application by Allen J bard and Larry R Faulkner.
- 17. Lithium-ion batteries basics and applications by Reiner Korthaneur.
- 18. Electrochemical supercapacitors: Scientific fundamentals and Technological applications, B.E. Conway.

#### SEMESTER - II

#### **MSCHE02C08: THEORETICAL CHEMISTRY - II**

#### Credit: 4

#### **TIME: 72 HOURS**

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Analyze the symmetry aspects of a given molecule and find its point group

CO 2. Explain the basic principles of group theory and construction of the character table

CO 3. Apply the principles of group theory to spectroscopy and chemical bonding

CO 4. Understand the interaction of matter with radiation in terms of the relation with the molecular energy levels.

CO 5. Explain and apply the selection rules pertaining to various molecular spectral transitions.

CO 6. Develop advanced awareness about the various spectroscopic techniques- IR, Raman, Electronic, and NMR

#### UNIT – I: MOLECULAR SYMMETRY, GROUPS, MATRICES 18 Hours

Symmetry elements and symmetry operations in molecules –point groups and their symbols – Classification of point groups– Systematic identification of point groups- order of a group- finite, Infinite, abelian, non-abelian, cyclic, and non-cyclic groups – sub-groups- Mathematical groups and its properties- group multiplication tables of  $C_{2v}$ ,  $C_{2h}$ , and  $C_{3v}$  –Rearrangement theoremclasses in a group and similarity transformation – Matrices – addition and multiplication of matrices – the inverse of a matrix- the character of a matrix- block diagonalization – matrix notation of symmetry operations –General expression for the character of an operationrepresentation of groups – construction of representation using vectors and atomic orbital as the basis –  $\Gamma$ cart, Representation generated by Cartesian coordinates positioned on the atoms of a molecule (H<sub>2</sub>O and SO<sub>2</sub> as examples) - $\Gamma$ regular – reducible and irreducible representations – construction of irreducible representation by reduction.

# UNIT II: THEORY OF MOLECULAR SYMMETRY AND APPLICATIONS OF GROUP THEORY 18 Hours

Great Orthogonality Theorem (GOT) (without proof) – Rules derived from GOT- construction of irreducible representation using GOT – construction of character tables (C<sub>2</sub>v, C<sub>2</sub>h, C<sub>3</sub>v, C<sub>4</sub>v). Four

areas of Character Table- Mulliken symbols- Reduction formula.

Applications of Group theory- Applications to chemical bonding – construction of hybrid orbitals – BF<sub>3</sub> CH<sub>4</sub>, PCI<sub>5</sub> as examples- Application to MO theory-. Group orbitals and their construction-Projection Operator method and pictorial method- Transition Moment Integral. Examples H<sub>2</sub>O, NH<sub>3</sub>, and octahedral complexes (sigma bonding using the pictorial method)

Applications in IR and Raman spectroscopy: symmetry aspects of molecular vibrations – Normal mode Analysis - selection rules for IR and Raman –-complementary character of 1R and Raman spectra – determination of the active 1R and Raman vibrational modes of H<sub>2</sub>O, NH<sub>3</sub>, CH<sub>4</sub>, BF<sub>3</sub>, N<sub>2</sub>F<sub>2</sub>

#### **UNIT - III: SPECTROSCOPY**

#### **18 Hours**

General theory: electromagnetic radiation, regions of the spectrum, the interaction of electromagnetic radiation with matter and its effect on the energy of molecules – Natural line width and broadening. The intensity of spectral lines – Einstein Coefficient- Rotational, vibrational, and electronic energy levels, and selection rules – transition moment integral

Microwave spectroscopy: Classification of molecules – rotational spectra of diatomic and polyatomic molecules – Rigid and non-rigid rotator models – Determination of bond lengths – isotope effect on rotation spectra – applications.

Vibrational and vibration – rotation spectra: Vibrational energies of diatomic molecules – the interaction of radiation with vibrating molecules – anharmonicity of molecular vibrations, fundamental, overtones and hot bands – Degree of freedom of polyatomic molecules and nature of molecular, vibrations (eg.  $CO_2$  and  $H_2O$ ). vibration – rotation spectra of diatomic and polyatomic molecules selection rules – determination of force constant.

Raman Spectroscopy: Theory of Raman spectra (classical and quantum mechanical theory) – pure rotational vibrational Raman spectra, vibrational –rotational Raman spectra, selection rules – mutual exclusion principle – Applications of Raman and I R spectroscopy in the elucidation of molecular structure (eg. H<sub>2</sub>O, N<sub>2</sub>O and CO<sub>2</sub> molecules)

#### UNIT -IV: SPECTROSCOPY II

#### **18 Hours**

Electronic spectra: Electronic spectra of diatomic molecules – vibrational coarse structure and rotational fine structure of electronic spectrum – Franck – Condon principle – Types of electronic transitions – Fortrat diagram – Dissociation and pre – dissociation – calculation of heat of dissociation.

Nuclear Magnetic Resonance Spectroscopy: General theory - magnetic properties of nuclei theory and measurement techniques - population of energy levels - solvents used -chemical shift and its measurement - factors affecting chemical shift - Nuclear resonance - Relaxation methods - integration of NMR signals - spin sin coupling - coupling constant j and factors affecting it - shielding and de shielding - chemical shift assignment of major functional groups - classification (AX, AB, ABX,) spin decoupling - Application to the study of simple molecules. REFERENCE

- 1. F A Cotton, "Chemical Applications of Group Theory" Wiley Eastern.
- 2. L H Hall "Group Theory and Symmetry in Chemistry", McGraw Hill.
- 3. V Ramakrishnan and M S Gopinathan, "Group Theory in Chemistry" Vishal Publications, 1992.
- 4. Banwell and Mc Cash "Fundamentals of Molecular Spectroscopy", Tata McGraw Hill
- 5. G Aruldas "Molecular Structure and Spectroscopy", Prentice Hall,
- 6. Manas Chanda "Atomic Structure and Chemicals Bonding including Molecular Spectroscopy, 4th Edn," Tata McGraw Hill
- 7. Barrow "Molecular Spectroscopy," McGraw Hill.
- 8. P W Atkins "Physical Chemistry," ELBS
- 9. S Swarna Lakshmi, T Saroja, and R M Ezhilarasi "A Simple Approach to Group Theory in Chemistry" - Universities Press
- 10. Thomas Engel "Quantum Chemistry and Spectroscopy" Pearson.

11. Quinn "Computational Quantum Chemistry - II: The Group Theory Calculator" - Ane Books

12. H.Kaur "Spectroscopy" 3rd Edition Pragati Prakashan Meerut

#### **MSCHE02C09: INORGANIC CHEMISTRY - II**

#### Credit: 4

#### **TIME: 72 HOURS**

**18 Hours** 

**18 Hours** 

**18 Hours** 

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1: Develop advanced knowledge about the VB and MO theory of coordination compounds CO 2: Explain the spectroscopic features of complexes and interpret the spectra of complexes CO 3: Describe the magnetic behaviour of complexes and apply magnetic properties in the structural determination of complexes

CO 4: Understand the various mechanisms operative in inorganic complexes during substitution and in electron transfer reactions.

CO 5: Explain different physical methods in Inorganic chemical analysis

#### UNIT - I: COORDINATION CHEMISTRY - I

Coordination numbers 2 to 12 and geometry – VB theory, assumption, and limitations. Crystal field theory of coordination compounds – d-orbital splitting in octahedral, tetrahedral, and square planar fields. Crystal field effect on ionic radii and lattice energies – Jahn Teller effect – evidence for ligand field splitting – spectrochemical series. MOT in coordination compounds – MO energy level diagrams for octahedral, tetrahedral, and square planar configuration with and without  $\pi$  bonding. Effect of  $\pi$ bonding in stability – nephelauxetic series – experimental evidence for metal-ligand. Covalent bonding in the complex. Comparison of three theories as applied to metal complexes.

#### UNIT - II: COORDINATION CHEMISTRY - II

Spectroscopic ground states – term symbols for d<sup>n</sup> ion. selection rules for d-d transitions – effect of spin-orbit coupling and vibronic coupling on electronic transitions - Orgel diagram of transition metal complexes( d<sup>1</sup> to d<sup>9</sup> configurations) Tanabe Sugano diagrams - Charge Transfer Spectra Magnetic behaviors – susceptibility, measurements – Gouy method diamagnetic corrections. Spin-only value – orbital contributions – spin-orbit coupling, ferro, and antiferro magnetic coupling – spin cross-over system – Temperature dependence of magnetic behaviour - Applications of magnetic measurements to structural determinations of transition metal complexes.

#### UNIT - III: COORDINATION CHEMISTRY III

The reaction of metal complexes: Stability constants - chelate effect - Irwing-Willian order of stability. Factors affecting the stability of metal complexes. Determination of binary formation

constants by pH meter and spectrophotometry - Job's Method - energy profile of a reaction

Reaction of complexes: Ligand substitution reactions (Square planar and octahedral complexes). Rates of ligand substitutions, classification of mechanisms. The nucleophilicity of the entering group, The shape of the transition states, The activation of octahedral complexes, Base hydrolysis, stereochemistry, and Isomerisation reactions. A brief study of redox reaction – Outer sphere and Inner sphere mechanism – Marcus -Husch Theory

#### UNIT-IV: PHYSICAL TECHNIQUES IN INORGANIC CHEMISTRY 18 Hours

Study of inorganic compounds by the following methods - Diffraction methods - X-ray diffraction, neutron diffraction

UV, IR, Raman Spectroscopic Methods, Resonance technique – nuclear magnetic resonance, electron paramagnetic resonance, Mossbauer spectroscopy

Ionization-based techniques – photon electron spectroscopy, x-ray absorption spectroscopy, mass spectrometry

Chemical analysis – atomic absorption spectroscopy, CHN Analysis, X-ray fluorescence elemental analysis

Magnetometry - electrochemical techniques

#### REFERENCE

- 1) S F A Kettle, Coordination Chemistry, Thomas Nelson and Sons
- 2) J C Bailer, Chemistry of coordination compounds, Reinhold
- 3) F Basolo R Johnson, Coordination Chemistry, Benjamin Inc
- 4) D Banergea, Coordination Chemistry, Tata McGraw Hill
- 5) D N Sathyanarayana, Electronic Absorption spectroscopy, and related techniques, Universities Press
- R Gopala and V N Ramalingam, Concise Coordination Chemistry, Vikas publishing house Pvt Ltd
- 7) M C Day and J Selbin, Theoretical Inorganic Chemistry, Affiliated EAST West Press
- 8) J E Huhee, Inorganic chemistry principles of structure and reactivity, Pearson Education India
- 9) R L Dutta and A Syamal, Elements of magneto chemistry, S Chand and Company Ltd
- 10) Glen E Rodgers, Inorganic and solid state chemistry, Cengage Learning
- R.S.Drago, Physical Methods in Chemistry, W.B.Saunders Company, Philadelphia, London, 1976.

#### MSCHE02C10: ORGANIC CHEMISTRY - II

#### Credit: 4

#### **TIME: 72 HOURS**

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Understand the basic concepts of conformational analysis and evaluate the effect of conformational changes in molecular reactions.

CO 2. Apply the basic concepts of stereochemistry in stereoselective asymmetric synthesis.

CO 3. Understand molecular orbital approaches in pericyclic reactions.

CO 4. Formulate mechanisms for pericyclic reactions and problems.

CO 5. Understand and analyze various name reactions in organic chemistry.

CO 6. Generate mechanisms for reactions and understand the basic concepts for asymmetric synthetic reagents.

#### **UNIT - 1: CONFORMATIONAL ANALYSIS**

#### (18 Hours)

(18 hours)

Difference between configuration and conformation. Internal factors affecting the stability of molecules – dipole interaction, bond opposition strain, bond angle strain. Conformational analysis of cyclic compounds: Cyclohexane Interconversion of axial and equatorial bonds in chair conformation of cyclohexane–the distance between the various H atoms and C atoms in chair and boat conformations.

Monosubstituted cyclohexane-methyl and t-butyl cyclohexanes-flexible and rigid systems. Conformation of substituted cyclohexanone, 2-bromocyclohexanone, dibromocyclo hexanone, (cis & trans), 2-bromo-4,4-dimethyl cyclohexanone. Anchoring group and conformationally biased molecules. Octant and axial and halo ketones rules. Stereochemistry of fused, bridged, and caged ring systems-decalins, norbornane, barrelene, and adamantanes.

#### **UNIT – 2: STEREOCHEMISTRY AND ASYMMETRIC SYNTHESIS**

Molecules with C, N, S based chiral centers. Axial, planar, and helical chirality with examples of R and S nomenclature using Cahn-Ingold-Prelog rules. Optical purity, enantiomeric excess, and diastereomeric excess and their determination. Topicity and pro stereoisomerism, prochiral centre, enantiotopic, homotopic, diastereotopic hydrogen atoms.

Asymmetric synthesis, need for asymmetric synthesis, stereoselectivity, and stereospecificity. Strategies in Asymmetric Synthesis: Chiral pool: Amino acids in the synthesis of benzodiazepinesconversion of L-tyrosine into L-Dopa; synthesis of beetle pheromone component (S)- (–)-ipsenol from (S)-(–)-leucine, Carbohydrates – (R) Sulcatol from 2-deoxy-D-ribose. Cram's rule, Cram's chelation control, Prelog's rule, and Felkin-Anh model.

#### **UNIT - 3: PERICYCLIC REACTIONS**

#### (18 Hours)

Symmetry properties of MOs – LCAO-MO theory of simple conjugated polyenes and cyclic polyenes – classification of pericyclic reactions- electrocyclic, cycloaddition, sigmatropic, chelotropic, and group transfer reactions. Mechanism and stereo course of electrocyclic, cyclo addition, and sigmatropic reactions.

Analysis of electrocyclic, cyclo addition, and Sigmatropic reactions by FMO, Woodward-Hoffmann Selection Rule, and Huckel-Mobius Method. Correlation diagram approach for electrocyclic, and cyclo addition reactions. Study of Electrocyclic Reactions: Nazarov cyclization. Study of Cycloaddition reactions: Stereo and Regiochemistry of Diels –Alder reaction, Intramolecular, Asymmetric, and retro Diels –Alder reaction. 1,3-dipolar cycloaddition, Ketene [2+2] cycloaddition. Sigmatropic reaction: [3,3] Cope rearrangement, Oxy-cope rearrangement, Aza cope rearrangement, classes, thia-claisen rearrangement, Fluxional molecules. [2,3] sigmatropic rearrangement, [5,5] sigmatropic reaction, metallo-ene reaction. Chelotropic reactions: (2+2) chemotropic cycloaddition, (4+2) chelotropic cycloaddition, stereochemistry of chelotropic reactions

#### **UNIT -4: ORGANIC REACTIONS AND REAGENTS**

#### (18 Hours)

Mannich, Simon-Smith, Heck, reactions. Michael, Prevost, and Woodward hydroxylation of alkenes, Shapiro reaction, Sharpless asymmetric epoxidation, ring formation by Dieckmann, Thorpe, and Acyloin condensation. Robinson ring annulations, reduction, and oxidation in synthesis – catalytic hydrogenation. Alkali metal reduction. Birch reduction. Wolff-Kishner reduction, Huang-Milon modification. Clemmenson reduction. LAH, DIBAL, sodium borohydride as reductance. Oppenauer oxidation. HIO<sub>4</sub>, OsO<sub>4</sub>, and mCPBA and their applications. Synthetic applications of the following reagents – Gillman's reagent, LDA, 1, 3 dithianes, DDQ, DDC, SeO<sub>2</sub>, Bakers yeast, NBS, Wilkinsons's catalyst. Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC2BH and IPCBH2. Reduction with CBH reagent.

#### References

1. E.L. Eliel, S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, 1994.

2. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 3/e, New Age

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Pub., 2010.

3. P. S. Kalsi, Stereochemistry, 4/e, New Age International Ltd.

4. P.S. Kalsi, Organic reactions & their mechanisms, 3/e revised, New Age International Ltd.

5. G. L. D. Krupadanam, Fundamentals of Asymmetric Synthesis, Universities Press, 2013.

6. S. Sankararaman, Pericyclic Reactions-A Textbook: Reactions, Applications and

Theory, Wiley VCH, 2005.

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

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

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

10. T. Landbery, Strategies, and Tactics in Organic Synthesis, Academic Press, London, 1989.

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

12. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford

University Press, 2004.

13. R.O.C.Norman&J.M.Coxon, Principles of Organic Synthesis, 3/e, Nelson Thornes

14. J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6/e, Wiley, 2007.

15. Modern methods of organic synthesis Carruthers,

16. H O House, Modern synthetic reactions

17. Fieser and Fieser, Reagent in organic synthesis

#### MSCHE02C11: PHYSICAL CHEMISTRY - II

#### Credit: 4

#### **TIME: 72 HOURS**

**18 Hours** 

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Apply the theory and methods of the statistical approach of thermodynamics.

CO 2. Analyze different classical and quantum mechanical distribution functions.

CO 3. Interpret classical and quantum statistical mechanics, including Boltzmann, Fermi-Dirac, and Bose-Einstein statistics.

CO 4. Illustrate band theory and the reciprocal lattice (k-space) formalism in terms of the crystal lattice.

CO 5. Analyze the theory of X-ray diffraction in solids.

CO 6. Develop an idea of different solid properties, focusing on electric and magnetic properties.

# **UNIT-1: STATISTICAL THERMODYNAMICS -I**

# Distinguishable and Indistinguishable particles, phase space, Ensemble, Macrostates, and microstates. Stirlings approximation- Thermodynamic probability --Derivation of Maxwell-Boltzmann distribution law - Partition function- physical significance- total partition function; Separation of Molecular partition function - Translational, Rotational, vibrational, electronic and nuclear partition function. Rotational temperature- Fundamental vibrational temperature-Thermal de-Broglie wavelength. Heat capacity of gases- Classical and quantum theories-Equipartition principle - Heat capacity of Hydrogen – Ortho and Para-Hydrogen. The atomic crystals: Einstein's theory of atomic crystal - Debye's modification of Einstein's model.

# UNIT-2: STATISTICAL THERMODYNAMICS -II AND QUANTUM STATISTICS 18 Hours

Partition function and thermodynamic functions- Partition function and equilibrium constants -Equation of state – Sackur Tetrode equation-Statistical formulation of the third law of thermodynamics.

Need for quantum statistics, Bose-Einstein statistics: Bosons-Bose Einstein distribution law, Bose-Einstein condensation, liquid helium, Fermi- Dirac statistics: Fermions- Fermi- Dirac distribution law, application to electrons in metals- Thermionic emission. Comparison of three statistics.

#### UNIT-3: IMPERFECTIONS IN SOLIDS AND CRYSTALLOGRAPHY

IMPERFECTIONS IN SOLIDS: Perfect and imperfect crystals, Classification; point defects, line and plane defects, vacancies- Thermodynamics and calculation of a number of defects of Schottky and Frenkel defects and formation of color centres, non-stoichiometric defects. Structures of FeO (Rock salt structure) and TiO<sub>2</sub>(anatase and rutile structure only)

CRYSTALLOGRAPHY: Isomorphism and polymorphism- Miller indices- diffraction of X-rays-Laue equation- Bragg's Law - - Bragg Method-Debye-Scherrer method of X-ray structure analysis of crystals, indexing of reflections, identification of unit cells from systematic absence in diffraction pattern-structure of simple lattice - X-Ray intensities-structure factor and its relation to intensity and electron density-phase problem.

#### **UNIT-4: PROPERTIES OF SOLIDS**

#### 18 Hours

**18 Hours** 

**Electronic structure of solids**-band theory and band structure of conductors, insulators, and semiconductors. Refinement to simple band theory - k-space and Brillouin Zones.

**Electrical properties**- electrical conductivity- Hall effect- dielectric properties- piezoelectricity-Ferroelectricity and conductivity.

**Magnetic properties-** diamagnetism- Lagevin theory of diamagnetism- paramagnetism- Ferri, antiferro and ferromagnetism.

Superconductivity in metals - BCS theory- Meissner effect -type I & II superconductors.

**Transition metal Oxides** –Structure of Spinels, Inverse-spinels, and Perovskites, application of perovskites in solar cells.

Solid state lighting: Organic Light Emitting Diodes (OLEDs) - Principle, Device Architecture, Advantages and Disadvantages.

Quasicrystals -Basic introduction and applications only.

#### REFERENCES

1. M.C. Gupta-"Elements of Statistical Thermodynamics-New age international.

2. L.K Nash-"Elements of Statistical Thermodynamics-Addision Wesley publishing.

3. Kistinand Sorfuran-"A course on statistical thermodynamic"-Academic 1971.

4. D.A.McQuarie-"Statistical thermodynamic"-HarperandRow1973.

5. D.K.Chakraharth-"Solid state chemistry"-New age publication.

6. I.V.Azaroof-"Introduction to solids"-McCrawHil.

7. Lesley E. Smart and Elaine A. Moore. "Solid state chemistry an introduction" Third edition, 2005. Taylor and Francis group. A.R.West, Solid State Chemistry and its Applications, (1984) John Wiley and Sons, Singapore
UriShmueli. "Theories and techniques of crystal structure determination" Oxford University Press, 10.2007.

10. Christopher Hammond. "The basics of crystallography and diffraction" Third edition, 2009, Oxford University Press.

11. Molewyn Hughes-"Physical chemistry"-Pergamon press. 24. S. Glasstone and H.S. Taylor-"Treatise of Physical Chemistry"-Dvan Nostrand.

12, Feridoun Samavat\*, Mohammad Hossein Tavakoli, Safdar Habibi, Babak Jaleh, Parisa Taravati Ahmad, *Open Journal of Physical Chemistry*, 2012, 2, 7-14 http://dx.doi.org/10.4236/ojpc.2012.21002

# MSCHE01&02C05: INORGANIC CHEMISTRY PRACTICAL- I (1<sup>st</sup> and 2<sup>nd</sup> semester)

#### **TIME: 108 HOURS**

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1: Identify advanced laboratory practices and develop laboratory skills through handson experiences.

CO 2: Identify the cations including rare elements, in a mixture of unknown salts

CO 3: Analyze metal ions using the volumetric method

CO 4: Analyze water quality parameters like hardness and DO

CO 5: Synthesize and characterize metal complexes of historical importance by various physicochemical methods

CO 6: Record, interpret and analyze UV-Vis and IR spectra, TG curves, and XRD patterns of different metal complexes

CO 7: Predict the spectral characteristics of a given metal complex.

#### **Course Content:**

**Part 1:** Separation and identification of four metal ions of which two are rare/less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo, and Li (interfering acid radicals not present). Confirmation by spot test. (Minimum 10 mixtures are to be recorded)

#### Part 2:

- 1) Volumetric estimation
  - a) EDTA Al, Ca, Cu, Ni, Co, Hardness of water
  - b) Cerimetry Fe(II), nitrate
  - c) Estimation of Dissolved Oxygen by Winkler's method
- 2) Preparation of the metal complexes, checking metal content and their characterization using UV-Vis spec / IR spec / TG & DTA /Magnetic susceptibility/ XRD data: Nickel (dimethyl glyoxime), Potassium trioxalatochromate (III), Tetraammoniumcopper (II) sulphate and Hexamminecobalt (III) chloride, and Potassiumhexathiocyanato chromate(III).

#### [A minimum of 16 experiments to be recorded]

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#### Credit: 2

#### REFERENCE

- 1) A. I. Vogel, A Text Book of Qualitative Inorganic Analysis, Longman 5th edition, 1979.
- 2) G H Jeffrey, J Bassette, J Mendham and R C Denny, Vogel's textbook of quantitative inorganic analysis, Longman, 1999
- 3) J. Derek Woollins, Inorganic Experiments, 3rd ed, Wiley, 2010
- 4) G S Vehla, Vogel's quantitative inorganic analysis (7th edition), Longman 2001
- D. A. Skoog and D. M. West, Analytical Chemistry: An Introduction, Saunders College Publishing, 4th edition, 1986.
- 6) W. G. Palmer, Experimental Inorganic Chemistry, Cambridge University,
- V. Ramanujam, Inorganic Semimicro Qualitative analysis, 3rd edition, The National Publishing Company, Chennai 1974.

# MSCHE01&02C06: ORGANIC CHEMISTRY PRACTICAL – I (1<sup>st</sup> and 2<sup>nd</sup> SEMESTER)

#### Time: 108 Hours

#### Credit: 2

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Develop hands-on laboratory experience in the separation and purification of organic compounds.

CO 2. Analyze organic compounds and acquire lab skills in the synthesis of organic compounds.

CO 3. Determine physical constants and purification techniques

CO 4. Develop skills in chromatography.

#### **Course Content**

#### 1) Analysis of organic binary mixtures (minimum 10 binary mixtures):

Separation of the binary mixture using physical and chemical methods. Checking its purity by Boiling points and Melting points. Preparation of the derivative of the compounds. The following types are expected:

(i) Solid-Solid (ii) Non-volatile liquid & Non-volatile liquid (iii) Water-soluble/insoluble solid and non-volatile liquid with compounds from the same or different chemical classes in all three categories.

#### 2) One-stage Preparation of organic compounds (minimum 10 compounds):

Single-stage preparation involving nitration, halogenation, oxidation, reduction, alkylation, acylation, condensation, and rearrangements. Prepare medicinally important compounds and Heterocyclic compounds.

Purify the synthesized compound by means of recrystallization.

Spot TLC, report the Rf value, and check the completion of the reaction and purity of the compound.

#### 3) Preparation of polymer compounds (minimum 3 compounds):

PMMA, Polystyrene, Polyesters, PANI (Exhibit during examinations)

#### **Books for Reference**

- 1. A I Vogel, A textbook of practical organic chemistry, Longman
- 2. A I Vogel, Elementary practical organic chemistry, Longman
- 3. F G Mann and B C Saunders, practical organic chemistry, Longman
- 4. Shriner and Others, Systematic identification of organic compounds
- 5. Dey, Sitharaman and Govindachari, A laboratory manual of organic chemistry
- 6. PR Singh, DC Gupta & KS Bajpai, Experimental organic chemistry vol I & II
- 7. Vishnoi, Practical organic chemistry
- 8. Fieser, Experiments in Organic chemistry

9. Joseph Sharma, Gunter Zweig, TLC and LC Analysis of international importance, Vol. VI and

VII, Academic Press

# MSCHE01&02C07: PHYSICAL CHEMISTRY PRACTICAL – I (I<sup>st</sup> and 2<sup>nd</sup> SEMESTER)

#### **Time: 108 Hours**

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Correlate and experimentally verify basic electrochemical principles related to conductance, mobility, and activities of ions

CO 2. Estimate concentration and molecular weights using cryoscopic methods

CO 3. Analyze physical constants like viscosity to determine the composition and molecular weights in the solution

CO 4. Perform electrochemical titrations in the laboratory by measuring the conductance and potential of solutions, and determination of dissociation constants of acids.

CO 5. Apply Physical chemistry concepts in the areas of phase equilibrium.

#### **Course Content**

#### 1) Conductivity experiments

Equivalent conductance of weak acids – verification of Ostwald's dilution law –calculation of dissociation constant

Equivalent conductance of strong electrolytes ( KCl). Verification of Onsagar equation

The activity coefficient of zinc in 0.002 M ZnSO4 using Debye-Huckel limiting law

Solubility product of sparingly soluble salts (AgCl-BaSO<sub>4</sub>)

Conductance titrations. HCl vs NaOH, (HCl+ HOAc) vs NaOH, AgNO3 vs KCl

#### 2. Solubility and Heat of solution

Heat of solution from solubility data – analytical method and graphical method (ammonium oxalate and succinic acid)

#### 3. Molecular weight determination

Molecular weight determination: Cryoscopic method and the transition temperature method. The molecular weight of a solid using a solid solvent by cooling curve method (solvents – naphthalene, biphenyl, diphenylamine, p-dichloro benzene). Molecular weight determination by the study of depression in transition temperature (sodium acetate, sodium thiosulphate, and strontium chloride)

#### 4. Cryoscopic study

Study of  $2KI + HgI_2 \rightarrow K_2HgI_4$  Reaction in water and determination of concentration of KI solution

#### 5. Refractometry

Determination of molar refraction of pure liquids (water, methanol, ethanol, chloroform, carbon

tetrachloride, glycerol). Determination of composition of mixture (alcohol-water, glycerol-water, KClwater)

#### 6. Viscosity

Determination of viscosity of pure liquids (water, methanol, ethanol, glycerol, benzene, nitrobenzene, carbon tetrachloride). Composition of the binary liquid mixture (benzene-nitrophenol, water-alcohol). Determination of molecular weight of a polymer (polystyrene in toluene)

#### 7. Potentiometry

The electrode potential of Zn and Ag electrodes in 0.1 M and 0.001 M solutions at 25 °C and determination of standard potentials. The mean activity coefficient of an electrolyte at different molalities by EMF method. Dissociation of the strength of the given HCl solution by the different potentiometric titration. Dissociation constant of acetic acid in DMSO, DMF, acetone, and dioxin by titrating with sodium hydroxide. Potentiometric titration. Acid-base titration, redox titration, and the mixture of HCl and HOAc.

#### 8. Phase rule

a) Solid and liquid equilibria: construction of phase diagram of simple eutectics, systems with congruent melting points, and solid solutions. Determination of the composition of unknown mixtures. Analytical and synthetic methods for the determination of solubilities and heat of solution

b) Partially miscible liquids: critical solution temperature, the influence of impurities on the miscibility temperature (KCl, NaCl, and /or succinic acid). Determination of the composition of unknown mixtures.

c) Completely miscible systems: construction of phase diagram of a two-component liquid system. Zeotropic and azeotropic

d) Three-component systems: with one pair of partially miscible liquids. Construction of phase diagrams of tie lines. Compositions of homogenous mixtures.

#### **REFERENCES:**

- 1. A Findlay and J A Kitchener, Practical physical chemistry, Longman
- 2. F Daniels and J H Mathews, Experimental physical chemistry, Longman
- 3. A M James, Practical physical chemistry, J A Churchill
- 4. H H Williard, L L Merritt and J A Dean, Instrumental methods of analysis, Affiliated East West press
- 5. D P Shoemaker and C W Garland, Experimental physical chemistry, McGraw Hill
- 6. W G Palmer, Experimental physical chemistry, Cambridge University Press
- (A minimum of 20 experiments to be recorded covering all units)

# MSCHE03&04C15: INORGANIC CHEMISTRY PRACTICAL – II (3<sup>rd</sup> and 4<sup>th</sup> SEMESTER)

#### **Time: 108 Hours**

#### Credit: 2

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Predict the methods for separation cations of a mixture

CO 2. Estimate metal ions present in a binary mixture following volumetric, gravimetric, and colorimetric methods

CO 3. Interpret data from an experiment, including constructing appropriate graphs and evaluating errors.

- CO 4. Analyze alloys and detect the cations present
- CO 5. Analyze trace metals using optical methods
- CO 6. Synthesize and characterize nanoparticles by various methods.

#### Course content:

- Quantitative separation of binary mixtures and estimation of components by volumetric, gravimetric, colorimetric, and electroanalytical methods Cu(II), Ni(II), Fe(III), Mg(II), Al(III), Ca(II), Ba(II) and Zn(II)
- 2) Analysis of ores
  - a) Analysis of brass
  - b) Analysis of solder
- 3) Synthesis of any two of the following metal oxide nanomaterials and their characterization using x-ray, microscopic or spectrochemical methods.
  - $ZnO / TiO_2 / Co_3O_4 / Co(OH)_2 / NiO / FeO etc. (Any two)$

#### [A minimum of 15 experiments to be recorded]

#### REFERENCE

- 1) G H Jeffrey, J Bassette, J Mendham and R C Denny, Vogel's textbook of quantitative inorganic analysis, ELBS Publication, London 1997
- 2) D M Adams and J B Raynor, Advanced practical inorganic chemistry, CRC Press, New York
- 3) W L Jolly, Preparative Inorganic reactions, Interscience Publishers, New York

- Textbook of Nanoscience and Nanotechnology, 2012 McGraw Hill Education (India) Private Limited By T Pradeep
- 5) Springer Handbook of Nanomaterials, by Robert Vajtai
- 6) Solution-Grown Zinc Oxide Nanowires, by Lori E. Greene, Benjamin D. Yuhas, Matt Law, David Zitoun, and Peidong Yang\*, Inorg. Chem. 2006, 45, 7535–7543

# MSCHE03&04C16: ORGANIC CHEMISTRY PRACTICAL – II (3<sup>rd</sup> and 4<sup>th</sup> SEMESTER)

#### **Time: 108 Hours**

#### Credit: 2

#### Course Outcomes: After the completion of the course, the learners should be able to

- CO 1. Develop lab skills in the extraction of natural compounds and qualitative analysis.
- CO 2. Synthesize and purify organic compounds
- CO 3. Develop skills in chromatographic techniques.
- CO 4. Analyze, examine, and solve spectral data.

#### **Course Contents:**

#### 1) Quantitative analysis and Extraction of natural products:

Estimation of the following

- i) Phenol (Using bromate-bromide mixture)
- ii) Aniline (Using bromate-bromide mixture)
- iii) Reducing sugars (using Fehling solution)
- iv) Iodine value of vegetable oil
- v) Saponification of vegetable oil
- vi) Estimation of ascorbic acid (Colorimetric method)
  - Extraction of natural compounds
- i) Caffeine from tea leaves, and ii) Casein from milk

# 2) Two-stage preparation of organic compounds (minimum 5 compounds):

- a) Preparation of p-nitroaniline from acetanilide:
- Acetanilide----p-nitroacetanilide----p-nitroaniline
- b) Preparation of Methyl orange from aniline:
- Aniline---sulphanilic acid---methyl orange
- c) Preparation of p-aminoazobenzene from aniline:
- Aniline---diazoaminobenzene---p-aminoazobenzene
- d) Preparation of m-nitroaniline from nitrobenzene:
- Nitrobenzene---m-dinitrobenzene---m-nitroaniline
- e) Preparation of Benzilic acid benzoin:

Benzoin----benzil----benzilic acid

f) Preparation of Benzanilide from benzophenone:

benzophenone---benzophenone oxime-benzanilide

g) Preparation of 2-phenyl indole from phenyl hydrazine:

Phenyl hydrazine----acetophenone phenyl hydrazone----2-phenyl indole

h) Preparation of caprolactam from cyclohexanone:

Cycohexanone----cyclohexanone oxime---Caprolactum

i) Preparation of m-nitrobenzoic acid from ethyl benzoate:

Ethyl benzoate----ethyl m-nitrobenzene----m-Nitrobenzoic acid

#### 3) Chromatographic Techniques:

Practical application of TLC:

a) Identification of food colours, amino acids, and sugars.

b) Identify the compound from the mixture of hydrocarbon and acids. (Compare using Rf values with the standard values)

c) Column chromatography in separating the exact amount of a given mixture of o-nitroaniline and pnitroaniline.

#### 4) Spectral evaluation of organic compounds:

Solving spectral problems from the standard textbooks by providing IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, and Mass spectra. (15 simple compounds only)

#### **Books for Reference**

1. A I Vogel, A Textbook of practical organic chemistry, Longmann

2. Elementary practical organic chemistry, part 3, quantitative organic analysis, Longmann

3. F G Mann and B C Saunders, Practical organic chemistry, Longman

4. PR Singh, DC Gupta & KS Bajpai, Experimental organic chemistry vol I&II

5. S Sadasivam and A Manickam, Biochemical methods, New Age International Publishers

6. J B Harbone, Phytochemical methods, Chapman and Hall, London

7. Joseph Sharma, Gunter Zweig, TLC and LC Analysis of international importance, Vol. VI and VII, Academic Press

8. Spectrometric Identification of Organic Compounds, Robert M. Silverstein, Francis X. Webster, David J. Kiemle, David L. Bryce, Wiley.

9. Organic Spectroscopy Principles, problems and their solutions, Jagadamba Singh and Jaya Singh, Pragati Edn.

10. Organic Spectroscopy Principles and Applications, Jag Mohan, Narosa Publishing House.

11. Organic Spectroscopy: Problems & Numericals, Dipti K Dodiya, Bluerose publishers.

12. Organic structures from spectra, 4th Edition, LD field, S Sternhell, JR Kalman, Wiley.

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# MSCHE03&04C17: PHYSICAL CHEMISTRY PRACTICAL – II (3<sup>rd</sup> and 4<sup>th</sup> SEMESTER)

#### **TIME: 108 Hours**

#### Credit: 2

#### Course Outcomes: After the completion of the course, the learners should be able to

CO 1. Experimentally analyze the concepts related to the kinetic aspects of chemical reactionsdetermination of concentration from graphs based on surface chemistry concepts

CO 2. Utilize stereochemical principles related to optical isomers to determine the concentration and kinetic parameters of specific reactions

CO 3. Apply UV-Visible spectroscopy to determine solution concentration, complex formation, equilibrium constant, metal ion concentration

CO 4. Perform basic spectral calculations and determination of specific parameters from UV-Visible spectroscopy and X-ray diffraction data

CO 5. Apply Computational chemistry to perform single-point energy calculation, geometry optimization, and Frontier orbital calculation at the HF level of theory

#### **Course Content:**

#### 1) Chemical kinetics

Acid hydrolysis of ester (methyl acetate or ethyl acetate) - determination of the given acids.

Acid Hydrolysis of ester - determination of Arrhenius parameters

Saponification of ethyl acetate – determination of specific reaction rate,  $K_2S_2O_8$ , and KI system Iodination of acetone in acid medium – determination of the order of reaction with respect to iodine and acetone

#### 2) Adsorption

Verification of Freundlich and Langmuir adsorption isotherms – charcoal-acetic acid system Determination of concentration of given acetic acid solution using the isotherms The same experiment using a charcoal-oxalic acid system

#### 3) Polarimetry

Determination of specific and molar optical rotations of glucose, fructose, and sucrose Determination of the concentration of a glucose solution Inversion of cane sugar in the Presence of HCl-Study of the Kinetics Determination of the specific rate of the reaction

Determination of the concentration of HCl

#### 4) Spectrophotometry

Verification of the Beer Lamberts law Determination of equilibrium constants of acid-base indicators Determination of concentration of a solution of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> (or KMnO<sub>4</sub>) Simultaneous determination of Mn and Cr in a solution of KMnO<sub>4</sub> and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> Investigation of complex formation between Fe(III) and thiocyanate

#### 5) Spectral analysis calculations

Determination of band gap/ HOMO/LUMO from UV Vis/CV analysis Determination of particle size/ Lattice parameters of Simple Cubic system from XRD

#### 6) Computational Chemistry Calculations

Single point energy calculations of simple molecules like H<sub>2</sub>O and NH<sub>3</sub> at the HF/3-21G level of theory.

The effect of the basis set on the single point energy of H<sub>2</sub>O and NH<sub>3</sub> using the Hartree-Fock method (3-21G, 6-31G basis sets can be used).

Geometry optimization of molecules like H<sub>2</sub>O, NH<sub>3</sub>, HCHO & C<sub>2</sub>H<sub>4</sub> at the HF/6-31G level of theory.

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

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

#### REFERENCES

- 1. F Daniels and J H Mathews, Experimental physical chemistry, Longmann
- 2. A M James, Practical physical chemistry, J A Churchill

3. H H Williard, L L Merit, and J A Dean, Instrumental methods of analysis, Affiliated East West Press

- 4. D P Shoemaker and C W Garland, Experimental physical chemistry, McGraw Hill
- 5. J B Yadav, Advanced practical physical chemistry, Goel Publishers
- 6. B Viswanathan, P S Raghavan, Practical physical chemistry, Viva Books Pvt Ltd
- 7. V D Athawale Parul Mathur, Experimental physical chemistry, New Age International

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Publishers

8. A Findlay and J A Kitchener, Practical physical chemistry, Longmann

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

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

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