

**GANDHI INSTITUTE OF TECHNOLOGY AND MANAGEMENT
(GITAM)
(Deemed to be University, Estd. u/s 3 of UGC Act 1956)**

VISA KHAPATNAM *HYDERABAD *BENGALURU
Accredited by NAAC with 'A+' Grade



REGULATIONS AND SYLLABUS

**Master of Science
In
Chemistry
(Specialization in Analytical and Organic Chemistry)**

(W.e.f. 2020-21 admitted batch)

Website: www.gitam.edu

M.Sc. in Chemistry
(Specialization in Analytical and Organic Chemistry)

REGULATIONS
(W.e.f. 2020-21 admitted batch)

1.0 ADMISSIONS

Admissions into M.Sc. Chemistry (Specialization in Analytical and Organic Chemistry) program of GITAM (deemed to be University) are governed by GITAM (deemed to be University) admission regulations.

2.0 ELIGIBILITY CRITERIA

- 2.1 A pass in B.Sc. with Chemistry as one of the Subject(s) and with a minimum aggregate of 50% marks in degree or any other equivalent Examination approved by GITAM (deemed to be University) .
- 2.2 Admissions into M.Sc. Chemistry (specialization in Analytical and Organic Chemistry) will be based on an All India GITAM Science Admission Test (GSAT) conducted by GITAM (deemed to be University) and the rule of reservation, wherever applicable.

3.0 CHOICE BASED CREDIT SYSTEM

Choice based credit system (CBCS) is introduced with effect from the admitted batch of 2015-16 based on UGC guidelines in order to promote:

- Student centered learning
- Cafeteria approach
- Inter-disciplinary learning.

Learning goals/objectives and outcomes are specified leading to what a student should be able to do at the end of the program.

4.0 STRUCTURE OF THE PROGRAMME

- 4.1 The program consists of:
- i) Core Courses (compulsory).
 - ii) Discipline centric electives which
 - a) are supportive to the discipline
 - b) give expanded scope of the subject
 - c) Give interdisciplinary exposure
 - d) Nurture the student skills
 - iii) Open electives are of general nature either related or unrelated to the discipline.
 - iv) Practical Proficiency Courses: Laboratory and Project work

- 4.2 Each course is assigned a certain number of credits depending upon the number of contact hours (lectures/tutorials/practical) per week.

- 4.3 In general, credits are assigned to the courses based on the following contact hours per week per semester.
- One credit for each lecture / tutorial hour.
 - One credits for two hours of practical.
 - Eight credits for project
- 4.4 The curriculum of four semesters M.Sc. Chemistry (specialization in Analytical and Organic Chemistry) program is designed to have a total of 91 credits for the award of M.Sc. degree.

5.0 MEDIUM OF INSTRUCTION:

The medium of instruction (including examinations and project reports) shall be English.

6.0 REGISTRATION

Every student has to register himself/herself for each semester individually at the time specified by the Institute / University.

7.0 ATTENDANCE REQUIREMENTS

- 7.1 A student whose attendance is less than 75% in all the courses put together in any semester will not be permitted to attend the end - semester examination and he/she will not be allowed to register for subsequent semester of study. He /She have to repeat the semester along with his / her juniors.
- 7.2 However, the Vice Chancellor on the recommendation of the Principal/ Director of the University College / Institute may condone the shortage of attendance to the students whose attendance is between 66% and 74% on genuine medical grounds and on payment of prescribed fee.

8.0 EVALUATION

- 8.1 The assessment of the student's performance in a Theory course shall be based on two components: Continuous Evaluation (40 marks) and Semester-end examination (60 marks).
- 8.2 A student has to secure an aggregate of 40% in the course in the two components put together to be declared to have passed the course, subject to the condition that the candidate must have secured a minimum of 24 marks (i.e. 40%) in the theory component at the semester-end examination.
- 8.3 Practical/ Viva voce/ Seminar etc. course are completely assessed under Continuous Evaluation for a maximum of 100 marks, and a student has to obtain a minimum of 40% to secure Pass Grade. Details of Assessment Procedure are furnished below in Table 1.

Table 1: Assessment Procedure

S. No.	Component of assessment	Marks allotted	Type of Assessment	Scheme of Examination
1	Theory	40	Continuous evaluation	(i) Three mid semester examinations shall be conducted for 15 marks each. The performance in best two shall be taken into consideration. (ii) 5 marks are allocated for quiz. (iii) 5 marks are allocated for assignments.
		60	Semester-end examination	The semester-end examination shall be for a maximum of 60 marks.
	Total	100		
2	Practicals	100	Continuous evaluation	60 marks for performance, regularity, record/ and case study. Weightage for each component shall be announced at the beginning of the semester. 40 marks (30 marks for experiment(s) and 10 marks for practical Viva-voce.) for the test conducted at the end of the Semester conducted by the concerned lab Teacher.
	Total	100		
3	Project work	200	Project evaluation	150 marks for evaluation of the project work dissertation submitted by the candidate. 50 marks are allocated for the project Viva-Voce. The project work evaluation and the Viva-Voce shall be conducted by one external examiner outside the University and the internal examiner appointed by the Head of the Department.

9. SUPPLEMENTARY EXAMINATIONS & SPECIAL EXAMINATIONS:

- 9.1 The odd semester supplementary examinations will be conducted on daily basis after conducting regular even semester examinations in April/May.
- 9.2 The even semester supplementary examinations will be conducted on daily basis after conducting regular odd semester examinations during November/December
- 9.3 A student who has completed his/her period of study and still has “F” grade in final semester courses is eligible to appear for Special Examination normally held during summer vacation.

10. PROMOTION TO THE NEXT YEAR OF STUDY

- 10.1 A student shall be promoted to the next academic year only if he/she completes the academic requirements of 60% of the credits till the previous academic year.
- 10.2 Whenever there is a change in syllabus or curriculum he/she has to continue the course with new regulations after detention as per the equivalency established by the BoS to continue his/her further studies

11. BETTERMENT OF GRADES

- 11.1 A student who has secured only a pass or second class and desires to improve his/her class can appear for betterment examinations only in 'n' (where 'n' is no. of semesters of the program) theory courses of any semester of his/her choice, conducted in summer vacation along with the Special Examinations.
- 11.2 Betterment of Grades is permitted 'only once', immediately after completion of the program of study.

12. REPEAT CONTINUOUS EVALUATION:

- 12.1 A student who has secured 'F' grade in a theory course shall have to reappear at the subsequent examination held in that course. A student who has secured 'F' grade can improve continuous evaluation marks upto a maximum of 50% by attending special instruction classes held during summer.
- 12.2 A student who has secured 'F' grade in a practical course shall have to attend Special Instruction classes held during summer.
- 12.3 A student who has secured 'F' grade in a combined (theory and practical) course shall have to reappear for theory component at the subsequent examination held in that course. A student who has secured 'F' grade can improve continuous evaluation marks upto a maximum of 50% by attending special instruction classes held during summer.
- 12.4 The RCE will be conducted during summer vacation for both odd and even semester students. Student can register a maximum of 4 courses. Biometric attendance of these RCE classes has to be maintained. The maximum marks in RCE be limited to 50% of Continuous Evaluation marks. The RCE marks are considered for the examination held after RCE except for final semester students.
- 12.5 RCE for the students who completed course work can be conducted during the academic semester. The student can register a maximum of 4 courses at a time in slot of 4 weeks. Additional 4 courses can be registered in the next slot.
- 12.6 A student is allowed to Special Instruction Classes (RCE) 'only once' per course.

13.0 GRADING SYSTEM

- 13.1 Based on the student performance during a given semester, a final letter grade will be awarded at the end of the semester in each course. The letter grades and the corresponding grade points are as given in Table-2.

Table 2: Grades & Grade Points

Sl.No.	Grade	Grade Points	Absolute Marks
1	O (outstanding)	10	90 and above
2	A+ (Excellent)	9	80 to 89
3	A (Very Good)	8	70 to 79
4	B+ (Good)	7	60 to 69
5	B (Above Average)	6	50 to 59

6	C (Average)	5	45 to 49
7	P (Pass)	4	40 to 44
8	F (Fail)	0	Less than 40
9	Ab. (Absent)	0	-

- 13.2 A student who earns a minimum of 4 grade points (P grade) in a course is declared to have successfully completed the course, and is deemed to have earned the credits assigned to that course, subject to securing a GPA of 5 for a Pass in the semester.

14.0 GRADE POINT AVERAGE

- 14.1 A Grade Point Average (GPA) for the semester/trimester will be calculated according to the formula:

$$\text{GPA} = \frac{\Sigma [C \times G]}{\Sigma C}$$

Where

C = number of credits for the course,

G = grade points obtained by the student in the course.

- 14.2 To arrive at Cumulative Grade Point Average (CGPA), a similar formula is used considering the student's performance in all the courses taken, in all the semesters up to the particular point of time.
- 14.3 CGPA required for classification of class after the successful completion of the program is shown in Table 3.

Table 3: CGPA required for award of Class

Distinction	$\geq 8.0^*$
First Class	≥ 7.0
Second Class	≥ 6.0
Pass	≥ 5.0

* In addition to the required CGPA of 8.0, the student must have necessarily passed all the courses of every semester in **first attempt**.

15.0 ELIGIBILITY FOR AWARD OF THE M.Sc. DEGREE

- 15.1 Duration of the program: A student is ordinarily expected to complete M.Sc. program in four semesters of two years. However a student may complete the program in not more than four years including study period.
- 15.2 However the above regulation may be relaxed by the Vice Chancellor in individual cases for cogent and sufficient reasons.
- 15.3 A student shall be eligible for award of the M.Sc Degree if he / she fulfill all the following conditions.

- a) Registered and successfully completed all the courses and projects.
- b) Successfully acquired the minimum required credits as specified in the curriculum corresponding to the branch of his/her study within the stipulated time.
- c) Has no dues to the Institute, hostels, Libraries, NCC / NSS etc, and
- d) No disciplinary action is pending against him / her.

15.4 The degree shall be awarded after approval by the Academic Council

15.0 Discretionary Power:

Notwithstanding anything contained in the above sections, the Vice Chancellor may review all exceptional cases, and give his decision, which will be final and binding.

**M.Sc. CHEMISTRY – Scheme of Instruction
I SEMESTER**

Sl. No.	Course Code	Name of the Course	Category	Credits	Scheme of Instruction			Scheme of Examination		
					Hours per Week		Total	Duration in Hrs.	Maximum Marks	
					L/T	P			Sem. End Exam	Con. Eval
1	SCY701	Inorganic Chemistry -I	PC	4	4	0	4	3	60	40
2	SCY703	Concepts of organic Chemistry	PC	4	4	0	4	3	60	40
3	SCY705	Chemical Kinetics and Thermodynamics	PC	4	4	0	4	3	60	40
4	SCY707	Molecular spectroscopy	PC	4	4	0	4	3	60	40
5	SSE 701/ SSE 703	Skill Enhancement Course*	SEC	2	0	3	3	3	--	100
6	VDC111	Venture Discovery	SEC	2	3	0	3	3	-	100
7	SCY721	Physical Chemistry Lab	PP	3	0	9	9	3	--	100
8	SCY723	Organic Chemistry Lab	PP	3	0	9	9	3	--	100
Total			---	26	16	21	37	--	240	460

*** SKILL ENHANCEMENT COURSE (CHOOSE ONE THE FOLLOWING)**

1. SSE 701: BASIC COMPUTER CONCEPTS
2. SSE 703: INFORMATION TECHNOLOGY TOOLS
3. PC – Program Core; PE – Program Elective; PP – Practical Proficiency;
OE – Open Elective CE – Continuous Evaluation; SE – Semester End

M.Sc. CHEMISTRY – Scheme of Instruction
II SEMESTER

Sl. No.	Course Code	Name of the Course	Category	Credits	Scheme of Instruction			Scheme of Examination		
					Hours per Week		Total	Duration in Hrs.	Maximum Marks	
					L/T	P			Sem. End Exam	Con. Eval
1	SCY 702	Inorganic chemistry-II	PC	4	4	0	4	3	60	40
2	SCY 704	Reaction mechanism and heterocyclic Compounds	PC	4	4	0	4	3	60	40
3	SCY 706	Electrochemistry and Surface Chemistry	PC	4	4	0	4	3	60	40
4	SCY 708	Quantum Chemistry and Group Theory	PC	4	4	0	4	3	60	40
5	SAE 702	Professional Communication Skills	AEC	2	0	3	3	3	--	100
6.	SCY 722	Inorganic Chemistry Lab	PP	3	0	9	9	3	--	100
7.	SCY 724	Computational Chemistry Lab	PP	3	0	6	6	3	--	100
Total			---	24	16	15	34	--	240	460

PC – Program Core; PE – Program Elective; PP – Practical Proficiency;
 OE – Open Elective CE – Continuous Evaluation; SE – Semester End

M.Sc. Chemistry (Specialization in Analytical Chemistry)– Scheme of Instruction
III SEMESTER

Sl. No.	Course Code	Name of the Course	Category	Credits	Scheme of Instruction			Scheme of Examination		
					Hours per Week		Total	Duration in Hrs.	Maximum Marks	
					L/T	P			Sem. End Exam	Con. Eval
1	SAC801	Concepts of Analytical Chemistry	PC	4	4	0	4	3	60	40
2	SAC803	Instrumental Methods of Analysis	PC	4	4	0	4	3	60	40
3	SAC805	Quality Assurance and Quality Control	PC	4	4	0	4	3	60	40
4	SOC801	Organic Synthesis	GE*(any one)	4	4	0	4	3	60	40
	SOC803	Organic Spectroscopy								
	SCY841	Green Chemistry								
	SCY 843	Chemistry of Nanomaterials								
5	SOE 801 to SOE XXX	OPEN ELECTIVE	OE*(any one)	3	3	0	3	3	60	40
6.	SAC 821	Electro analytical Techniques Lab	PP	3	0	9	9	3	--	100
7.	SCY 821	Chromatographic Separation and Spectroscopy Lab-I	PP	3	0	6	6	3	--	100
Total			---	25	19	15	34	--	300	400

M.Sc. CHEMISTRY (Specialization in Organic Chemistry) – Scheme of Instruction
III SEMESTER

Sl. No.	Course Code	Name of the Course	Category	Credits	Scheme of Instruction			Scheme of Examination		
					Hours per Week		Total	Duration in Hrs.	Maximum Marks	
					L/T	P			Sem. End Exam	Con. Eval
1	SOC801	Organic Synthesis	PC	4	4	0	4	3	60	40
2	SOC 803	Organic Spectroscopy	PC	4	4	0	4	3	60	40
3	SOC 805	Pericyclic Reactions and Photochemistry	PC	4	4	0	4	3	60	40
4	SAC803	Instrumental Methods of Analysis	GE*(any one)	4	4	0	4	3	60	40
	SAC805	Quality Assurance and Quality Control								
	SCY841	Green Chemistry								
	SCY 843	Chemistry of Nanomaterials								
5	SOE 801 to SOE XXX	OPEN ELECTIVE	OE*(any one)	3	3	0	3	3	60	40
6.	SOC 821	Multistage Synthesis Lab	PP	3	0	9	9	3	--	100
7.	SCY 821	Chromatographic Separation and Spectroscopy Lab-I	PP	3	0	6	6	3	--	100
Total			---	25	19	15	34	--	300	400

M.Sc. (Specialization in Analytical Chemistry)– Scheme of Instruction
IV SEMESTER

Sl. No.	Course Code	Name of the Course	Category	Credits	Scheme of Instruction			Scheme of Examination		
					Hours per Week		Total	Duration in Hrs.	Maximum Marks	
					L/T	P			Sem. End Exam	Con. Eval
1	SAC802	Separation Methods of Analysis	PC	4	4	0	4	3	60	40
2	SAC842	Analysis of Ores, Alloys and other materials	GE*(any one)	4	4	0	4	3	60	40
	SAC844	Pharmaceutical Analysis								
	SAC846	Environmental and Industrial material analysis								
3	SAC822	Quantitative Analysis Lab	PP	3	0	9	9	3	--	100
4	SCY822	Chromatographic Separation and Spectroscopy Lab-II	PP	3	0	6	6	3	--	100
5	SCY 892	PROJECT WORK	PP	8	0	0	0	3	--	200
Total			---	22	08	15	23	--	120	480

M.Sc. CHEMISTRY (Specialization in Organic Chemistry) – Scheme of Instruction
IV SEMESTER

Sl. No.	Course Code	Name of the Course	Category	Credits	Scheme of Instruction			Scheme of Examination		
					Hours per Week		Total	Duration in Hrs.	Maximum Marks	
					L/T	P			Sem. End Exam	Con. Eval
1	SOC802	Chemistry of Natural Products	PC	4	4	0	4	3	60	40
2	SOC 842	Bioorganic chemistry	GE*(any one)	4	4	0	4	3	60	40
	SOC 844	Medicinal Chemistry								
	SOC 846	Asymmetric Synthesis								
3	SOC 822	Qualitative Analysis Lab	PP	3	0	9	9	3	--	100
4	822	Chromatographic Separation and Spectroscopy Lab-II	PP	3	0	6	6	3	--	100
5	SCY 892	PROJECT WORK	PP	8	0	0	0	3	--	200
Total			---	22	08	15	23	--	120	480

M.Sc. CHEMISTRY - I SEMESTER
SCY 701: INORGANIC CHEMISTRY-I

Hours per week: 4
Credits: 4

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Course objectives:

- ❖ To obtain an introductory knowledge of bonding in coordination compounds
- ❖ To understand the magnetic properties and colour of coordination compounds
- ❖ To understand the basic spectroscopic properties of compounds
- ❖ To acquire a knowledge in stability of metal complexes in solutions
- ❖ To obtain a detailed knowledge in mechanisms of ligand substitution and electron transfers in coordination complexes

UNIT-I

Metal-ligand bonding: Isomerism in coordination compounds, Crystal field theory - crystal field splitting patterns in octahedral, tetrahedral, tetragonal, square planar, square pyramidal and trigonalbipyramidal geometries - Determination of crystal field splitting energy - calculation of crystal field stabilization energies - Factors affecting crystal field splitting energies-spectrochemical series. Ligand field theory - Molecular Orbital theory, MLCT and LMCT transitions in coordination compounds- Jahn-Teller effect.

Learning Outcomes: By the end of this unit, the student will be able to

- understand the bonding and structures of complex compounds
- learn how to calculate the crystal field energies

UNIT-II

Electronic spectra: Term symbols - spin-orbit coupling, Russell – Saunders coupling - derivation of term symbols for various configurations. Spectroscopic ground states, selection rules, correlation diagrams - Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1 - d^9 states), calculations of Dq , B and β parameters, charge transfer spectra.

Introduction to Mossbauer Spectroscopy: Mossbauer theory and parameters. Gamma radiation source, nuclear interactions (Isomer shift, quadrupole splitting, Magnetic hyperfine splitting), Applications in inorganic complexes (Bonding and Structure of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+}).

Learning Outcomes: By the end of this unit, the student will be able to

- understand the spectroscopic properties of compounds
- predict the suitable method to characterize the inorganic compounds by Mossbauer

UNIT-III

Metal-Ligand Equilibria in solutions: Stepwise and overall formation constants and their interaction, trends in successive formation constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, the chelate effect, determination of formation constants by pH metry and spectrophotometry. The Irving-Williams series.

Learning Outcomes: By the end of this unit, the student will be able to

- learn the solution chemistry principles
- understand the influence of metal and ligand on stabilization of complexes

UNIT-IV

Mechanisms of Inorganic Reactions-I: Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, Substitution reactions in octahedral complexes- kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, anation reactions, reactions without metal ligand bond cleavage.

Substitution reactions in square planar complexes, the trans effect in Pt(II) complexes, Polarisation and π -bonding theories of trans effect.

Learning Outcomes: By the end of this unit, the student will be able to

- learn the reactivity and kinetics of coordination complexes
- analyze the various types of substitution reactions

UNIT –V

Mechanisms of Inorganic Reactions-II: Oxidation-reduction reactions, classification of redox reactions, mechanism of one electron transfer reactions, Inner sphere redox reactions, outer sphere redox reactions, mixed inner and outer sphere reactions, two equivalent-one equivalent reactions of thallium (III)-thallium(I) and Hg(I)-Hg(II).

Learning Outcomes: By the end of this unit, the student will be able to

- learn the kinetics in electron transfer reactions of coordination complexes
- distinguish between ligand transfer and electron transfer reactions

Text Books

- 1) Advanced Inorganic Chemistry by F.A.Cotton and R.Wilkinson, VI Edition, Johnwilly and sons, New York, 2007.
- 2) Inorganic Chemistry: Principles of Structure and Reactivity by James E. Huheey, Okhil K. Medhi Ellen A. Keiter, Richard L. Keiter, 2006.
- 3) Inorganic Chemistry, Gary L. Miessler and D. A. Tarr, 3rd Edition 2004, Pearson-Prentice Hall.
- 4) Mechanisms of Inorganic Reactions in solution by D.Benson, McGraw Hill, London, 1968.
- 5) Mechanisms of Inorganic reactions: A study of metal complexes in solutions, F. Basalo& R. G. Pearson, Wiley-Eastern Pvt Ltd., 2ndEdn.
- 6) Kinetics and Mechanisms of reactions of Transition metal complexes by Ralph G. Wilkins, Wiley-VCH, Verlag GmbH & Co., 2002.
- 7) Mössbauer Spectroscopy by N.N. Greenwood and T.C. Gibb, Springer, 2011

M.Sc. CHEMISTRY - I SEMESTER
SCY703: CONCEPTS OF ORGANIC CHEMISTRY

Hours per week: 4
Credits: 4

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Preamble

This course is designed to explain the students about Nature of bonding in Organic Molecules, reactive intermediates; Stereochemistry and Stereoisomerism; Addition Mechanisms; various rearrangements; importance of some Natural Products

Course Objectives:

- To explain Nature of bonding in Organic Molecules, Concept of aromaticity, types of organic reactions and reactive intermediates
- To explain Stereochemistry and Stereoisomerism: Conformational/ Optical/ geometrical isomerism
- To explain Addition to carbon-carbon multiple bonds orientation and stereochemistry
- To explain various rearrangements: general mechanistic treatment to rearrangements
- To explain Isolation, structure elucidation and synthesis of some important Natural Products

UNIT- I

Nature of bonding in Organic Molecules: Localised and delocalised covalent bond, concept of aromaticity annulenes and hetero annulenes, inductive and mesomeric effects. Huckel's rule for aromaticity in benzenoid and non-benzenoid compounds, anti-aromaticity and homo-aromaticity. Introduction to types of organic reactions and reactive intermediates.

Learning Outcome

At the end of the unit, the student will be able to understand:

- inductive, mesomeric effects in organic molecules
- aromaticity, homo/anti-aromaticity in various benzenoid and non-benzenoid systems
- types of organic reactions
- reactivity and stability of reactive intermediates

UNIT- II

Stereochemistry and Stereoisomerism: Conformational isomerism and analysis in acyclic and simple cyclic systems - substituted ethanes, cyclopentane, cyclohexane, cycloheptane, cyclooctane and decalins. Optical isomerism - optical activity -molecular dissymmetry and chirality (Chiral centre, chiral axis, chiral plane), elements of symmetry. Fisher's projection D,L. and R,S. configurations - relative and absolute configurations, optical isomerism due to asymmetric carbon atoms, optical isomerism in biphenyls, allenes and spirans. Optical isomerism of nitrogenous compounds, racemisation and resolution - geometrical isomerism and E,Z configurations, properties of geometrical isomers. Recognition of symmetry elements and chiral structures, R-S-nomenclature, diastereoisomerism in acyclic and cyclic systems inter conversions of Fisher, Newman and Saw-horse projections.

Learning Outcome

At the end of the unit, the student will be able to learn

- Conformational isomerism, analysis in acyclic and simple cyclic systems,
- D,L. and R,S. configurations,
- Optical isomerism
- E,Z configurations, R-S-nomenclature
- Fisher, Newman and Saw-horse projections

UNIT- III

Addition Mechanisms: Addition to carbon-carbon multiple bonds. Addition reactions involving electrophiles, nucleophiles and free radicals, cyclic mechanisms, orientation and stereochemistry.

Learning Outcome

At the end of the unit, the student will be able to learn about Addition Mechanisms of

- carbon-carbon multiple bonds involving
- electrophiles,
- nucleophiles,
- free radicals, and their rules

UNIT- IV Rearrangements: Classification and general mechanistic treatment of nucleophilic, free radical and electrophilic rearrangements, Wagner–Meerwein, Tiffeneau–Demjanov rearrangement, Neber, Hofmann, Stevens, Wittig and Fries rearrangements.

Learning Outcome

At the end of the unit, the student will be able to learn **the** Mechanisms of rearrangement:

- Wagner–Meerwein,
- Tiffeneau–Demjanov,
- Neber, Hofmann,
- Stevens ,Wittig and Fries rearrangements

UNIT- V

Natural Products: Isolation, structure elucidation and synthesis of alkaloids: atropine, nicotine, papaverine, purines: caffeine. flavonoids: quercetin: genestein. terpenoids: citral , α - terpineol, camphor.

Learning Outcome

At the end of the unit, the student will be able to know the importance of

- alkaloids: atropine, nicotine, papaverine
- purines: caffeine
- flavonoids: quercetin, genestein;
- terpenoids: citral , α - terpineol, camphor

Textbooks:

1. Organic Chemistry, Vol. I (Sixth Edn), and Vol. II (Fifth Ed.), by I.L.Finar, ELBS, 2002
2. Organic Chemistry (Fifth Edn.)by Morrison and Boyd, PHI, India, 2011
3. Organic Chemistry by Mukherjee, Singh and Kapoor, Vols, I and II, Wiley Eastern., 2010
4. Reaction Mechanism in Organic Chemistry by Mukherjee and Singh, Macmillan India., 2012
5. Advanced Organic Chemistry by Jagdamba Singh and L D S Yadav,Pragati Edition., 2010
6. Organic reactions, Stereochemistry, and Mechanism, P.S. Kalasi, New Age International,2007

Reference Books:

1. Advanced Organic Chemistry by Jerry March (3rd Edn.) Wiley Eastern, 2006
2. Stereochemistry of carbon compounds by E.Eliel. McGraw Hill, 2008
3. A guide book to mechanism in Organic Chemistry by Peter Sykes, ELBNS, 1986

M.Sc. CHEMISTRY - I SEMESTER
SCY705: CHEMICAL KINETICS AND THERMODYNAMICS

Hours per week: 4

Semester End Examination: 60 Marks

Credits: 4

Continuous Evaluation: 40 marks

Preamble:

Chemical kinetics explains about theories Arrhenious, reaction coordinates transition state, thermodynamic formulation of reaction rates. It emphasis on Reactions in solution- primary and secondary salt effects, effect of solvent on reaction rate; effect of substituents on reaction rates. Thermodynamics describes macroscopic behavior of a system in a time-invariant state in terms of bulk properties such as pressure, volume, temperature and chemical potential. It is also concerned with the potential functions obtained by combining these properties and their relation to spontaneity of physical and chemical processes.

Course Objectives:

- To provide insights into the concept of Collision theory, Arrhenious equation, .
- To introduce the idea of Unimolecular reactions- Lindemann's theory and RRKM theory
- To demonstrate the laws of thermodynamics through real-life examples and applications
- To generate an intuitive understanding among the students for the concept of entropy and its relevance in design of a heat engine
- To demonstrate how thermodynamics dictates the feasibility of physical transformations and chemical reactions

Chemical Kinetics

UNIT –I

Theories of reaction rates- Collision theory, Arrhenious equation; Theory of absolute reaction rates-Reaction coordinate, transition state, thermodynamic formulation of reaction rates; Unimolecular reactions- Lindemann's theory and RRKM theory; Reactions in solution- primary and secondary salt effects, effect of solvent on reaction rate; effect of substituents on reaction rate - Hamett and Taft equations with examples - Linear Free Energy relations.

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Theories of reaction rates, collision theory, transition state theory.
- thermodynamic formulation of reaction rates, Reactions in solution- primary and secondary salt effects, effect of solvent on reaction rate.
- Hamett and Taft equations with examples - Linear Free Energy relations.

UNIT –II

Catalysis: Homogeneous catalysis- acid-base catalysis- mechanism of acid-base catalysis - Enzyme catalysis- Michaelis-Menten kinetics - Heterogeneous catalysis- Langmuir adsorption isotherm- unimolecular and bimolecular reactions-catalytic poisoning-active centers, surface area-determination of surface area with BET equation.

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Homogeneous catalysis- acid-base catalysis- mechanism of acid-base catalysis - Enzyme catalysis

- Unimolecular and bimolecular reactions-catalytic poisoning-active centers

UNIT –III

Complex reactions: Opposing, parallel and consecutive reactions (all first order type)- derivation of rate-law, Chain reactions- derivation of rate-laws for $\text{H}_2\text{-Cl}_2$ and $\text{H}_2\text{-Br}_2$ reactions; Fast reactions-study of fast reactions by flow methods and relaxation methods.

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Opposing, parallel and consecutive reactions
- Chain reactions- derivation of rate-laws for $\text{H}_2\text{-Cl}_2$ and $\text{H}_2\text{-Br}_2$ reactions
- Fast reactions-study of fast reactions by flow methods and relaxation methods

Thermodynamics

UNIT –IV

Second law of thermodynamics- concept of entropy-entropy change in reversible process and irreversible process-entropy of mixing; Fugacity: concept-Determination- Variation of fugacity with pressure; concept of partial molar properties- chemical potential-significance-variation with pressure and temperature- Gibbs-Duhem equation; Van't Hoff reaction isotherm, Clausius-Claperyon equation.

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Concept of entropy-entropy change in reversible process and irreversible process.
- Fugacity: concept-Determination- Variation of fugacity with pressure; concept of partial molar properties- chemical potential.
- Gibbs-Duhem equation; Van't Hoff reaction isotherm, Clausius-Claperyon equation.

UNIT –V

Third law of thermodynamics- Nernst heat theorem-determination of absolute entropy-limitations of third law of thermodynamics; Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, Partition function-rotational, translational, vibrational and electronic partition functions for diatomic molecules.

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Nernst heat theorem-determination of absolute entropy-limitations of third law of thermodynamics.
- Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics.
- Partition function-rotational, translational, vibrational and electronic partition functions for diatomic molecules

Text Books:

1. Chemical Kinetics, K. J. Laidler, 3rd. Ed, Pearson education (Singapore) Pte. Ltd., New Delhi, 2004
2. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan India, 1993
3. A text book of Physical Chemistry, 3rd edition, Vol. 2, 3 and 5, K.L.Kapoor, Macmillan, India Limited, 2012
4. Physical Chemistry – P. W. Atkins, Oxford University press, VIIth edition, 2002.
5. Thermodynamics A Core Course- R. C. Srivastava, S. K. Saha and A. K. Jain, Prentice-Hall of India, II Edition, 2004.

M.Sc. CHEMISTRY - I SEMESTER
SCY707: MOLECULAR SPECTROSCOPY

Hours per week: 4
Credits: 4

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Preamble:

Molecular spectroscopy explains the definition of electromagnetic radiation, different regions of spectrum, polarization of light; plane of vibration, plane of polarization, optical activity, factors effecting the angle of rotation, specific rotation, optical rotator dispersion and circular dichroism, cotton effect. It emphasis on Vibrational and rotational Spectroscopy, Raman effect- Classical and quantum mechanical explanations, Electronic spectra of diatomic molecules- vibrational course structure- intensity of spectral lines- Franck-Condon principle. It deals with the basic ideas about instrument, use of NMR in medical diagnostics, advantages of FT NMR, and Basic principles of ESR, zero field splitting-factors affecting the 'g' value.

Course Objectives:

- To provide insights of Electromagnetic radiation- interaction of electromagnetic radiation with matter.
- To explain Rotational spectra of diatomic molecules- rigid rotor-selection rules- calculation of bond length.
- To describe the chemical shift and its measurements, factor influencing chemical shift, deshielding, spin-spin interaction.
- To understand basic principles, zero field splitting-factors affecting the 'g' value.

UNIT-I

Spectroscopy-Unifying Principles: Electromagnetic radiation- interaction of electromagnetic radiation with matter- absorption, emission, transmission, reflection, refraction, dispersion and scattering Polarization: polarization of light; plane of vibration, plane of polarization, optical activity, factors effecting the angle of rotation, specific rotation, optical rotator dispersion and circular dichroism, cotton effect .

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Definition of electromagnetic radiation- interaction of electromagnetic radiation with matter,
- Factors effecting angle of rotation, specific rotation, optical rotator dispersion and circular dichroism, cotton effect.

UNIT-II

Vibrational and rotational Spectroscopy: Rotational spectra of diatomic molecules- rigid rotor-selection rules- calculation of bond length- isotopic effect-second order stark effect and its applications, infrared spectra of diatomic molecules-harmonic and anharmonic oscillators- Selection rules- overtones-combination bands-calculation of force constant-anharmonicity constant and Zero point energy . Fermi resonance, simultaneous vibration-rotation spectra of diatomic molecules.

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Rotational spectra of diatomic molecules, rigid rotor-selection rules.
- second order stark effect and its applications, infrared spectra of diatomic molecules- harmonic and anharmonic oscillators

UNIT-III

Raman Spectroscopy: Raman effect-Classical and quantum mechanical explanations- pure rotational, vibrational and vibrational-rotational Raman spectra-selection rules, mutual exclusion principle.

Electronic Spectroscopy: Electronic spectra of diatomic molecules- vibrational course structure- intensity of spectral lines- Franck-Condon principle – applications- rotational fine structure –band head and band shading- charge transfer spectra.

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Raman effect, Classical and quantum mechanical explanations- pure rotational, vibrational and vibrational-rotational Raman spectra.
- Electronic spectra of diatomic molecules- vibrational course structure- intensity of spectral lines- Franck-Condon principle – applications.

UNIT-IV

Nuclear Magnetic Resonance Spectroscopy: Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factor influencing chemical shift, deshielding, spin-spin interaction, factor influencing coupling constant 'J'. spin decoupling, basic ideas about instrument, use of NMR in medical diagnostics, advantages of FT NMR.

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements
- factor influencing coupling constant 'J'. spin decoupling, basic ideas about instrument, use of NMR in medical diagnostics, advantages of FT NMR.

UNIT-V

Electron Spin Resonance Spectroscopy: Basic principles, zero field splitting-factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants- experimental technique - applications of ESR studies:deuterium,methyl free radical,benzene free radical,parabenzosemiquinone,copper phthalocyanine,chloroform,hemoglobin, glycine and alanine,

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Basic principles, zero field splitting-factors affecting the 'g' value.
- Experimental technique - applications of ESR studies.

Text Books:

1. C.N. Banwell and E.M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4th edition, Tata McGraw Hill, New Delhi, 1994
2. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill, 1962
3. Instrumental Methods of Chemical Analysis, Willard, Meritt, Dean & Settle(Wiley Eastern), 7th Ed., 1988

M.Sc. CHEMISTRY - I SEMESTER
SSE 701: BASIC COMPUTER TOOLS

Hours per week: 3

Examination: 100 Marks

Credits: 2

Preamble: The course gives an understanding about the characteristics and classification of computers, various components of computer along with different operating systems that are available. It gives a hands on training on the packages MS-Word, MS-Power Point and MS-Excel. The course also comprehends AI tools.

Basics of Computers: Definition of a Computer - Characteristics and Applications of Computers – Block Diagram of a Digital Computer – Classification of Computers based on size and working – Central Processing Unit – I/O Devices, Primary, Auxiliary and Cache Memory – Memory Devices. Software, Hardware, Firmware and People ware – Definition and Types of Operating System – Functions of an Operating System – MS-DOS –MS Windows, UNIX. Introduction to AI tools.

MS-Word

Features of MS-Word – MS-Word Window Components – Creating, Editing, ormatting and Printing of Documents – Headers and Footers – Insert/Draw Tables, Table Auto format – Page Borders and Shading – Inserting Symbols, Shapes, Word Art, Page Numbers, Equations – Spelling and Grammar – Thesaurus – Mail Merge.

MS-PowerPoint

Features of PowerPoint – Creating a Blank Presentation - Creating a Presentation using a Template - Inserting and Deleting Slides in a Presentation – Adding Clip Art/Pictures -Inserting Other Objects, Audio, Video- Resizing and Scaling of an Object –Slide Transition – Custom Animation.

MS-Excel

Overview of Excel features – Creating a new worksheet, Selecting cells, Entering and editing Text, Numbers, Formulae, Referencing cells – Inserting Rows/Columns –Changing column widths and row heights, auto format, changing font sizes, colors, shading.

Reference Books:

1. Fundamentals of Computers by V.RajaRaman, PHI Learning Pvt. Ltd, 2010.
2. Microsoft Office 2010 Bible by John Walkenbach, Herb Tyson, Michael R. Groh andFaihe Wempen, Wiley Publications, 2010.

Learning Outcomes:

- Able to understand fundamental hardware components that make up a computer's hardware and the role of each of these components
- Understand the difference between an operating system and an application program, and what each is used for in a computer.
- Acquire knowledge about AI tools.
- Create a document in Microsoft Word with formatting that complies with the APA guidelines.
- Write functions in Microsoft Excel to perform basic calculations and to convert number to text and text to number.
- Create a presentation in Microsoft PowerPoint that is interactive and legible content

SSE 703 : INFORMATION TECHNOLOGY TOOLS

Hours per week: 3

Examination: 100 Marks

Credits: 2

Preamble: The course enables the student to understand networking concepts related to Internet and introduce the social Networking sites and working of Email. It gives orientation of Block Chain technology. It give hands on training in SPSS, R Programming and creation of simple HTML documents.

Introduction to Internet: Networking Concepts, Data Communication –Types of Networking, Internet and its Services, Internet Addressing –Internet Applications–Computer Viruses and its types –Browser –Types of Browsers.

Internet applications: Using Internet Explorer, Standard Internet Explorer Buttons, Entering a Web Site Address, Searching the Internet– Introduction to Social Networking: twitter, tumblr, Linkedin, facebook, flickr, skype, yahoo!, google+, youtube, WhatsApp, etc.

E-mail : Definition of E-mail, Advantages and Disadvantages, User Ids, Passwords, Email Addresses, Domain Names, Mailers, Message Components, Message Composition, Mail Management, Email Inner Workings.

WWW-Web Applications, Web Terminologies, Web Browsers ,URL–Components of URL, Searching WWW –Search Engines and Examples.

Block Chain technology: What is Block Chain, Blockchain Architecture, How Block chain Transaction Works? Why do we need Blockchain? Block chain versions, Block chain Variants, Block chain Use Cases, Important Real-Life Use Cases of Block chain Bitcoin cryptocurrency: Most Popular Application of Block chain, Block chain vs. Shared Database, Myths about Block chain, Limitations of Block chain technology.

SPSS : SPSS Commands, Descriptive Statistics, Hypothesis Testing, Test of Difference, Analysis of Variance- One Way ANOVA, Non Parametric Tests, Correlation Analysis, Regression Analysis.

R Programming: Becoming familiar with R, Working with Objects, Introduction to Graphical Analysis.

HTML: WEB Terminology, Structure of HTML Document, HTML – Head and Body tags, Semantic tags- HR- Heading, Font, Image & Anchor tags, Different Types of Lists using Tags, Table Tags, Image Formats – Creation of Simple HTML Documents.

Reference Books:

- In-line/On-line : Fundamentals of the Internet and the World Wide Web by Raymond Greenlaw and Ellen Hepp, 2nd Edition, TMH.
- Microsoft Office 2010 Bible by John Walkenbach, Herb Tyson, Michael R. Groh and Faithe Wempen, Wiley Publications.

Learning Outcomes:

- Enable to understand the basic networking concepts, types of networks, Internet Explorer and www.
- Outline the Block chain architecture, Bitcoin Crypto currency and Limitations of Block Chain.
- Choose different statistical tests to be performed on the data sets.
- Demonstrate the R programming with simple graphs.
- To make use of commands to structure HTML document.

VDC111 : Venture Discovery

Hours per week: 3

Examination: 100 Marks

Credits: 2

Course description and learning outcomes

India as part of its Make in India initiative has been focusing on creating incubation centers within educational institutions, with an aim to generate successful start-ups. These start-ups will become employment creators than employment seekers, which is the need of the hour for our country.

This common course for all the disciplines is a foundation on venture development. It is an experiential course that lets students venture and find out what is a business, financial and operating models of a business are. How to design and prototype a solutions that meets their customers' needs and generate revenue for the business.

LEARNING OBJECTIVES

- Discover who you are – Values, Skills, and Contribution to Society.
- Gain experience in actually going through the innovation process.
- Conduct field research to test or validate innovation concepts with target customers.
- Understand innovation outcomes: issues around business models, financing for start-ups, intellectual property, technology licensing, corporate ventures, and product line or service extensions.

On successful completion of this course, students will be able to:

	Learning Outcome	Assessment
1	Understand conceptual framework of the foundation of a venture	A1, A2
2	Understand the concept of purpose, mission and value-add service offered by a venture	A3
3	Analyze design and positioning of the product	A3
4	Demonstrate prototyping	A3
5	Analyze business, revenue and operating models	A3

Course outline and indicative content

Unit I (6 sessions)

Personal Values: Defining your personal values, Excite & Excel, Build a Team, Define purpose for a venture. Four stages: Personal Discovery, Solution Discovery, Business Model Discovery, Discovery Integration.

Unit II (6 sessions)

Solution Discovery: Craft and mission statement, Experience design, Gaining user insight, Concept design and positioning, Product line strategy, Ideation & Impact.

Unit III (6 sessions)

Business Model Discovery: Prototyping solutions, Reality Checks, Understand your industry, Types of business models, Define Revenue Models, Define Operating Models

Unit IV (6 sessions)

Discovery Integration: Illustrate business models, Validate business models, Define company impact

Unit V (6 sessions)

Tell a Story: Can you make money, Tell your venture story.

Assessment methods

Task	Task type	Task mode	Weightage (%)
A1. Assignments	Individual	Report/Presentation	20
A2. Case / Project/Assignment	Groups* or Individual	Presentations/Report/Assignment	40
A3. Project	Individual/Group	Report/Pitch	40

Transferrable and Employability Skills

	Outcomes	Assessment
1	Know how to use online learning resources: G-Learn, online journals, etc.	A1 & A2
2	Communicate effectively using a range of media	A1 & A2
3	Apply teamwork and leadership skills	A2
4	Find, evaluate, synthesize & use information	A1 & A2
5	Analyze real world situation critically	A3
6	Reflect on their own professional development	A3
7	Demonstrate professionalism & ethical awareness	A2
8	Apply multidisciplinary approach to the context	A2

Learning and teaching activities

Mixed pedagogy approach is adopted throughout the course. Classroom based face to face teaching, directed study, independent study via G-Learn, case studies, projects and practical activities (individual & group)

Teaching and learning resources

Soft copies of teaching notes/cases etc. will be uploaded onto the G-learn. Wherever necessary, printouts, handouts etc. will be distributed in the class. Prescribed text book will be provided to all. However you should not limit yourself to this book and should explore other sources on your own. You need to read different books and journal papers to master certain relevant concepts to analyze cases and evaluate projects. Some of these reference books given below will be available in our library.

Prescribed Modules:

Access to NU-IDEA online modules will be provided.

Referential text books and journal papers:

Personal Discovery Through Entrepreneurship, Marc H. Meyer and Chaewon Lee, The Institute of Enterprise Growth, LLC Boston, MA.

Suggested journals:

Vikalpa, Indian Institute of Management, Ahmedabad
Journal of General Management, Mercury House Business Publications, Limited
Harvard Business Review, Harvard Business School Publishing Co. USA

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M.Sc. CHEMISTRY - I SEMESTER
SCY721: PHYSICAL CHEMISTRY LAB

Hours per week: 9

Credits: 3

Semester End Examination: 60 Marks

Continuous Evaluation: 40 marks

Preamble:

This lab course complements the theory course in physical chemistry by providing a hands-on experience in performing conductometric and potentiometric titrations. It provides complete experience in performing pH metry involving strong and weak acids and bases and also to understand the applications of pH metric titrations. It gives an idea about phase separation and effect of electrolyte on the system. An exhaustive emphasis on chemical kinetics is covered.

Course Objectives:

- To know about the practical idea about different phases, followed by the effect of electrolyte on phase equilibrium.
- To demonstrate how cell constant and equivalent conductance can be determined from conductance measurements
- To demonstrate the differences between the conductometric titrations involving strong and weak acids and bases
- To demonstrate the usefulness of potentiometric titrations in determining the endpoint of redox titrations.
- To understand the applications of pH metric titrations.
- To get an idea about distribution coefficient and kinetics of potassium iodide system.
 1. Critical solution temperature of phenol -water system
 2. Effect of electrolyte (NaCl) on miscibility temperature
 3. Comparison of acid strengths through acid catalyzed methyl acetate hydrolysis
 4. Conductometric titration of a strong acid with strong base
 5. Conductometric titration of a weak acid with strong base
 6. Conductometric titration of a mixture of weak and strong acid with strong base
 7. Distribution coefficient of I_2 between two immiscible solvents.
 8. Equilibrium constant of $KI + I_2 \leftrightarrow KI_3$ by distribution method.
 9. Potentiometric titration of redox system (ferrous ammonium sulfate with $K_2Cr_2O_7$).
 10. Determination of composition of cuprammonium cation.
 11. Determination of strength of strong acid using pH meter.
 12. Determination of strength of weak acid using pH meter.

Learning Outcomes:

By the completion of these experiments, the student will be able to

- Understand critical solution temperature of Phenol water system, effect of electrolyte.
- Understand the concepts of conductance and electrode potential
- Understand the principles of conductometric and potentiometric measurements
- Obtain hands-on experience in performing conductometric and potentiometric titrations and gain knowledge of their applications.

Text Books

1. Practical physical Chemistry, B. Viswanadham and P.S. Raghavan, Viva Books pvt. Ltd., New Delhi, 2005
2. Advanced practical physical Chemistry, J. B Yadav, Goel Publishing house, Meerut, 1998.

**M.Sc. CHEMISTRY - I SEMESTER
SCY723: ORGANIC CHEMISTRY LAB**

Hours per week: 9
Credits: 3

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Preamble:

This lab course complements the theory course in organic chemistry by providing a hands-on experience in performing basic laboratory techniques. It provides complete experience of synthesis of compounds involving two steps along with functional group analysis.

Course Objectives:

- To learn simple laboratory techniques
- To learn synthesis of organic compounds in two steps
- To identify functional groups of given organic compounds

(1).Organic laboratory techniques, synthesis of organic compounds involving 2 stages.

(2) Systematic Organic Qualitative identification of about six compounds containing one or two functional groups by chemical reactions

Learning outcomes:

By the completion of these experiments, the student will be able to

- simple laboratory techniques: m.p., b.p., distillation, recrystallization
- synthesis of organic compounds in two steps
- analyse the functional groups of given organic compounds by adopting Systematic organic qualitative analysis procedure

Text books:

1.Vogel's Textbook of Practical Organic Chemistry By B S Furniss, A.J. Hannaford, Peter W.G. Smith, A.R.Tatchell,5th Edition, Pearson Publication

M.Sc. CHEMISTRY - II SEMESTER
SCY702: INORGANIC CHEMISTRY-II

Hours per week: 4
Credits: 4

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Course objectives:

- ❖ *To obtain an introductory knowledge of bioinorganic Chemistry and Inorganic medicinal compounds*
- ❖ *To obtain a detailed knowledge in catalytical applications of organometallic compounds.*
- ❖ *To acquire a knowledge in structure and bonding of inorganic cluster compounds*
- ❖ *To learn the bonding in solid state structures*
- ❖ *Understand the basic aspects of Nanoscience & Nanomaterials*

UNIT-I

Bioinorganic Chemistry: Metal ions in Biology; Molecular mechanism of ion transport across membranes- ionophores; Photosynthesis; Nitrogen fixation; Oxygen uptake proteins - hemoglobin and myoglobin; Electron transfer proteins - Cytochromes and Ferredoxins; Inorganic medicinal compounds - superoxide dismutase mimics, vanadium based diabetic drugs and platinum containing anticancer agents.

Learning Outcomes: By the end of this unit, the student will be able to

- *learn the role of metal ions in biological systems*
- *understand the role of various enzymes and proteins in biological systems*
- *acquire the knowledge in biomedical applications of inorganic compounds*

UNIT-II

Organometallic Chemistry: Introduction, Nomenclature, the 18-electron rule. Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand; Metallocenes-ferrocene; Catalysis by organometallic compounds - hydrogenation, hydroformylation, and polymerization.

Learning Outcomes: By the end of this unit, the student will be able to

- *learn the structure and bonding in organometallic compounds*
- *understand the catalytical applications of various organometallic compounds*

UNIT-III

Metal Clusters: Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal compounds with metal-metal multiple bonds. Preparation, properties and structures of $\text{Re}_2\text{Cl}_8^{2-}$, $\text{Mo}_2\text{Cl}_8^{4-}$, $\text{Re}_2(\text{RCOO})_4\text{X}_2$, $\text{Cr}_2\text{Cl}_9^{3-}$, $\text{W}_2\text{Cl}_9^{3-}$, Re_3Cl_9 , $\text{Re}_3\text{Cl}_{12}^{3-}$, $\text{Mo}_6\text{Cl}_8^{4+}$, $\text{Nb}_6\text{Cl}_{12}^{2+}$.

Learning Outcomes: By the end of this unit, the student will be able to

- *understand the structure and bonding metal clusters*
- *learn the relation between structure and bonding in metal clusters*

UNIT-IV

Solid State and Structural Chemistry: Crystal structures - close packing, body centered and primitive structures; Symmetry in crystals, Crystallographic point groups; Description of structures - AB structures (NaCl, CsCl, ZnS), AB₂ structures (Rutile, Fluorite), A₂B₃ structures (β -Al₂O₃), ABO₃ structures (perovskite) and AB₂O₄ Spinels.

Learning Outcomes: *By the end of this unit, the student will be able to*

- *acquire the knowledge in solid state chemistry*
- *learn the structure and bonding in crystal structures of various solid state materials*

UNIT V

Chemistry of Nanomaterials: Classification – zero, one and two dimensional nanomaterials. Synthesis and biomedical applications of gold, silver and iron oxide nanoparticles, Introduction to fullerenes and carbon nanotubes (SWCNTs, MWCNTs). Synthesis, Properties and applications of CNTs.

Learning Outcomes: *By the end of this unit, the student will be able to*

- *understand basic information regarding nanoscience and types of various nanomaterials*
- *identify various methods for synthesis of nanomaterials and its applications*

Text Books

1. Bioinorganic Chemistry by L. Bertini, H.B. Gray, J.S. Valentine, Uni. Science Books, 1994.
2. Bioinorganic Chemistry: A short course by Rosette M. Roat-Malone, John-Wiley Sons. Inc., 2002.
3. Inorganic Chemistry: Principles of Structure and Reactivity by James E. Huheey, Okhil K. Medhi Ellen A. Keiter, Richard L. Keiter, 2006.
4. Inorganic Chemistry, Gary L. Miessler and D. A. Tarr, 3rd Edition 2004, Pearson-Prentice Hall.
5. Synthesis of Inorganic Materials by Ulrich Schubert and Nicola Husing, Wiley-VCH, 2000
6. Textbook of Nanoscience and Nanotechnology by B.S. Murthy, Universities Press, 2012
7. 'Nanochemistry: A chemical approach to Nanomaterials', Ozin Geoffrey A. and Andre C. Arsenault, Royal Society of Chemistry Publication, 2005.

M.Sc. CHEMISTRY - II SEMESTER
SCY704: REACTION MECHANISM AND HETEROCYCLIC COMPOUNDS

Hours per week: 4
Credits: 4

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Preamble

This course is designed to explain Aliphatic and Aromatic Substitution Reactions; Elimination Reactions, basic concepts of some organic Name reactions; Synthesis and Reactivity of heterocycles containing one or two heteroatoms

Course Objectives:

- To explain Aliphatic and Aromatic Substitution Reactions
- To explain Elimination Reactions
- To explain basic concepts of some organic Name reactions
- To explain Synthesis and Reactivity of the compounds with one heteroatom
- To explain Synthesis and Reactivity of the compounds with more than one heteroatom

UNIT-I

Aliphatic and Aromatic Substitution Reactions: Nucleophilic - The S_N2 , S_N1 , S_Ni and SET mechanisms, neighbouring group participation, anchimeric assistance, classical and non classical carbocations, phenonium ions, norbornyl system, allylic, aliphatic, trigonal and vinylic carbon, factors effecting substitutions. Electrophilic - $SE1$, $SE2$ and SEi Mechanisms and related effects.

Learning Outcome

At the end of the unit, the student will be able to understand the mechanisms and related effects of S_N2 , S_N1 , S_E^1 , S_E^2 , NGP

UNIT-II

Elimination Reactions: The $E2$, $E1$ and $E1cB$ mechanisms and their orientation of the double bond. Reactivity-effects of substrate structure, attacking base, leaving group and the medium. Stereochemistry of eliminations in acyclic and cyclic systems, orientation in eliminations – Saytzeff and Hoffman elimination, Regio and stereo selectivity reactions.

Learning Outcome

At the end of the unit, the student will be able to learn mechanisms, Stereochemistry, orientation in eliminations: Saytzeff and Hoffman rules in $E2$, $E1$ and $E1cB$

UNIT-III

Basic concepts of some organic reactions: Aldol, Stobbe, Cannizaro, Wittig, Grignard, Reformatsky Reactions. Openauer oxidation, Clemmensen reduction, Birch reductions, Michael addition, Mannich Reaction, Diels - Alder reaction, Ene-reaction, Bayer -Villiger Reaction, Wolf-Kishner reduction, Favorskii reaction, Chichibabin reaction. Vilsmeier, Robinson annulation.

Learning Outcome

At the end of the unit, the student will be able to understand the mechanisms and application of Aldol, Stobbe, Cannizaro, Wittig, Grignard, Reformatsky Reactions. Openauer oxidation; Clemmensen/ Birch/ Wolf-Kishner reduction, Michael addition, Mannich/ Diels – Alder/ Ene/ Bayer -Villiger/Favorskii/Chichibabin/ Vilsmeier reaction, Robinson annulation

UNIT-IV

Synthesis and Reactivity of the compounds with one heteroatom: Pyrrole, Furan, Thiophene, Pyridine, Quinoline, Isoquinoline, Indole, Benzofuran and Benzothiophene.

Learning Outcome

At the end of the unit, the student will be able to understand Chemistry of Pyrrole, Furan, Thiophene, Pyridine, Quinoline, Isoquinoline, Indole, Benzofuran and Benzothiophene

UNIT-V

Synthesis and Reactivity of the compounds with more than one heteroatom Pyrazole, Imidazole, Oxazole, Isoxazole, Thiazole, Isothiazole, Pyridazine, Pyrimidine, Pyrazine and Purine.

Learning Outcome

At the end of the unit, the student will be able to understand Chemistry Pyrazole, Imidazole, Oxazole, Isoxazole, Thiazole, Isothiazole, Pyridazine, Pyrimidine, Pyrazine and Purine

Text books:

1. Organic Chemistry Vol. I (Sixth Edn.) and Vol. II (Fifth Edn.) by I.L. Finar ELBS., 2002
2. Organic Chemistry (fifth Edn.) by Morrison and Boyd, PHI, India., 2011
3. Reaction Mechanism in Organic Chemistry by Mukherjee Singh, Macmillan, India., 2012
4. Heterocyclic compounds by Raj K Bansal, New age International, 1999
5. Reaction Mechanism & Reagent in Organic Chemistry, G.R. Chatwal, Himalaya Publishing House, 2012.

Reference Books:

1. Advanced Organic Chemistry by Jerry March (3rd Edn.) Wiley Eastern., 2006
2. Organic Chemistry (fifth edition) by Francis A. Carey Tata Mac Graw Hill publishing company Limited, New Delhi, 2007

M.Sc. CHEMISTRY - II SEMESTER
SCY706: ELECTROCHEMISTRY AND SURFACE CHEMISTRY

Hours per week: 4
Credits: 4

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Preamble:

In “**ELECTROCHEMISTRY AND SURFACE CHEMISTRY**” electro chemistry deals with conversion of electrical energy to chemical energy and how free energy change of a spontaneous chemical reaction can be converted into EMF. It is concerned with how EMF measurements enable determination of free energy and equilibrium constants of a chemical reaction. Surface chemistry deals with chemisorption, Langmuir and Freundlich isotherms. BET equation (derivation not required) and surface area determination.

Course Objectives:

- To introduce Measurement of EMF-Nernst equation-effect of complexation on electrode potential.
- To introduce the concepts of ionic mobility, Importance of over-voltage; Activity and activity coefficients- determination of mean ionic activity coefficient by EMF method.
- To demonstrate the applications of Batteries-primary and secondary cells – leclanche cell, lead acid storage battery, Nickel-Cadmium cell; Fuel cells-Oxygen-hydrogen fuel cell
- To discuss concept of Surface active agents- classification- critical micellar concentration (CMC)-factors affecting the CMC of surfactants- determination of CMC.
- To discuss Basic concepts- monomers, repeat units, degree of polymerization, linear, branched and network polymers, classification of polymers

ELECTROCHEMISTRY

UNIT-I

Electrochemical cells: Measurement of EMF-Nernst equation-effect of complexation on electrode potential; Polarization-Decomposition potential and overvoltage- Factors affecting overvoltage- Importance of over-voltage; Activity and activity coefficients- determination of mean ionic activity coefficient by EMF method; Debye-Huckel limiting law (DHLL) and its verification, Extended Debye-Huckel law; Debye-Huckel-Onsager equation(derivation not required)-verification and its limitations.

Learning Outcomes:

By the end of this Unit, the student will be able to

- Grasp concepts of electrochemistry
- Activity and activity coefficients- determination of mean ionic activity coefficient by EMF method

UNIT-II

Applications: Batteries-primary and secondary cells – leclanche cell, lead acid storage battery, Nickel-Cadmium cell; Fuel cells-Oxygen-hydrogen fuel cell; Corrosion- theories of dry and wet corrosion-different forms of corrosion-prevention and control of corrosion - cathodic protection-sacrificial anodic and impressed current methods- inhibitors-anodic and cathodic inhibitors; protective coatings-galvanising and tinning.

Learning Outcomes:

By the end of this Unit, the student will be able to learn

- Concepts of Batteries-primary and secondary cells, Fuel cells-Oxygen-hydrogen fuel cell
- cathodic protection-sacrificial anodic and impressed current methods
- Protective coatings-galvanising and tinning.

SURFACE CHEMISTRY

UNIT-III Adsorption

Gibbs adsorption isotherm, types of adsorption isotherms, physisorption and chemisorption, Langmuir and Freundlich isotherms. BET equation (derivation not required) and surface area determination. Kinetics of surface reactions involving adsorbed species, Langmuir-Hinshelwood mechanism.

Learning Outcomes:

By the end of this Unit, the student will be able to learn

- Gibbs adsorption isotherm, types of adsorption isotherms, physisorption and chemisorptions.
- Langmuir and Freundlich isotherms. BET equation.
- Kinetics of surface reactions involving adsorbed species.

UNIT-IV Micelles

Surface active agents- classification- critical micellar concentration (CMC)-factors affecting the CMC of surfactants- determination of cmc. Solubilisation-factors influencing the solubilisation. Micellization-thermodynamics of micellization. Micro emulsions-comparison of microemulsions with conventional emulsions-applications. Reverse micelles.

Learning Outcomes:

By the end of this Unit, the student will be able to learn

- Surface active agents- classification
- Critical micellar concentration (CMC)-factors affecting the CMC of surfactants.
- Emulsions-applications. Reverse micelles

UNIT-V Polymer chemistry

Basic concepts- monomers, repeat units, degree of polymerization, linear, branched and network polymers, classification of polymers. Polymerization-Free radical, ionic and co-ordination polymerization. Kinetics of condensation (step-growth), free-radical and ionic polymerizations. Physical characterization: Number and mass average molecular weights (M_n , M_w), Determination of molecular masses – Osmometry, viscometry and light scattering methods.

Learning Outcomes:

By the end of this Unit, the student will be able to learn

- Basic concepts- monomers, repeat units, degree of polymerization
- Kinetics of condensation (step-growth), free-radical and ionic polymerizations
- Osmometry, viscometry and light scattering methods.

Text Books:

1. Physical Chemistry – P. W. Atkins, Oxford University press, VII edition, 2002.
2. Physical Chemistry of macromolecules- D. D. Deshpande, Vishal Publications.
3. Micellar Catalysis (Surfactant Science series vol.133), Mohammad Niyaz Khan. Taylor and Francis, 2007
4. Micelles, Theoretical and applied aspects., V. Moroi, Plenum press, New York, 1992

5. A text book of Physical Chemistry Vol. 2,3 and 5 K.L.Kapoor, Macmillan, India Limited, 2004

M.Sc. CHEMISTRY - II SEMESTER
SCY708: QUANTUM CHEMISTRY AND GROUP THEORY

Hours per week: 4
Credits: 4

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Preamble:

Quantum Chemistry deals with behaviour of matter at atomic and sub-atomic dimensions with particular emphasis on the electronic structure that profoundly influences the feasibility and progress of any chemical reaction. Group theory is concerned with symmetry present in molecules and how symmetry enables prediction of molecular properties.

Course Objectives:

- To introduce the concept of wave-particle duality, fundamental axioms of quantum theory and significance of Schrodinger wave equation.
- To illustrate applications of Schrodinger equation to simple model systems and establish their connection to realistic atomic and molecular systems;
- To demonstrate ideas underlying various approximation methods in dealing with multi-electron systems and necessity of making such approximations
- To provide a quantum mechanical perspective of chemical bonding through various modern theories like Valence Bond Theory and Molecular Orbital Theory
- To introduce molecular symmetry and group theory and provide insights into its applications in chemical problems

Course Outcomes:

- Understand the necessity of axioms and wave equation in describing electrons
- Acquaintance with methodologies for solving Schrodinger equation for simple systems
- Insights into various approximation methods and necessity of approximations in problem solving
- Appreciate the idea that existence of chemical bond is a quantum mechanical effect
- Insights into usefulness of symmetry arguments in solving chemical problems

UNIT-I

Wave equation-interpretation of wave function-properties of wave function-normalization and orthogonalisation, operators-linear and non linear, commutators of operators. Postulates of quantum mechanics, setting up of operators, observables - Hermitian operator-Eigen values of Hermitian operator, Particle in one dimensional box.

Learning Outcomes:

By the end of this Unit, the student will be able to

- Understand the concepts of wave-particle duality, uncertainty and probability

- Appreciate the necessity of postulates of quantum mechanics and significance of wave equation in describing electrons
- Apply particle in 1D box to model π -electrons in open chain conjugated molecules

UNIT-II

Particle in a three dimensional box, rigid rotor, wave mechanics of systems with variable potential energy- simple harmonic oscillator- solution of wave equation-selection rules, qualitative discussion of hydrogen atom (expressions for wavefunction and energy).

Learning Outcomes:

By the end of this Unit, the student will be able to

- Understand how different types of molecular motions can be modeled quantum mechanically using simple model systems
- Appreciate the fact that exact solution of wave equation is possible only for one-electron systems
- Grasping the idea that a multi-electron system in the crudest approximation can be considered as a combination of one-electron systems

UNIT-III

Approximation methods: Perturbation theory- application to ground state energy of Helium atom; Variation principle (statement only), Many electron atom-Hartree-Fock Self consistent field method (qualitative treatment only).

Learning Outcomes:

By the end of this Unit, the student will be able to

- Understand the necessity of making approximations for multi-electron systems
- Appreciate the mathematical ideas involved in approximation methods
- Apply approximation methods to simple systems
- Compare and contrast perturbation and variational methods and evaluate the relevance of each method in solving a given chemical problem

UNIT-IV

Bonding in molecules: Born-Oppenheimer approximation- Hydrogen molecule ion, LCAO-MO and VB treatments of the hydrogen molecule (fundamental concepts only); electron density, forces and their role in chemical bonding. Hybridization and valence MOs of H_2O , NH_3 and CH_4 . Huckel π -electron theory and its applications to ethylene, 1,3-butadiene and benzene.

Learning Outcomes:

By the end of this Unit, the student will be able to

- Understand the mathematics behind modern theories of chemical bonding
- Apply Huckel's π -electron theory to simple molecules
- Compare and contrast Valence Bond Theory and Molecular Orbital Theory

UNIT-V

Symmetry and Group Theory in Chemistry: Symmetry elements and symmetry operations and point groups, Schoenflies symbols, classification of molecules into point groups, Axioms of group theory, group multiplication tables for C_{2v} and C_{3v} point groups, representations-reducible and irreducible representations, Mulliken symbols, orthogonality theorem (without proof and its implications), Character table and its anatomy.

Learning Outcomes:

By the end of this Unit, the student will be able to

- Understand different symmetry elements and operations present in molecules
- Classify molecules into different point groups based on symmetry
- Generating representations for a given basis in a molecule and reducing it into smaller dimensions
- Apply character tables to predict feasibility of spectroscopic transitions

Text Books:

1. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill, 4th Ed., 1994
2. Quantum Chemistry, Donald A. McQuarrie, Viva Student Ed., Viva Books Pvt. Ltd., New Delhi, 2013.
3. Quantum Chemistry, I.N. Levine, 5th Ed., Pearson Educ. Inc., New Delhi, 2000
4. Physical Chemistry: A Molecular Approach, D.A. Mc Quarrie and J.D. Simon, Viva Books, New Delhi, 1998
5. Symmetry and Spectroscopy of Molecules, K.Veera Reddy, New Age, 1988

M.Sc. CHEMISTRY - II SEMESTER
SAE 702 PROFESSIONAL COMMUNICATION SKILLS

Hours per week: 3

Continuous Evaluation: 100 Marks

Credits: 2

Preamble

This course is designed to expose students to the basics of academic and professional communication in order to develop professionals who can effectively apply communication skills, theories and best practices to meet their academic, professional and career communication needs.

Objectives :

To enable students to

- acquaint themselves with basic English grammar
- acquire presentation skills
- develop formal writing skills
- develop creative writing skills
- keep themselves abreast with employment-readiness skills

UNIT - I

BACK TO BASICS: Tenses, Concord – Subject Verb Agreement, Correction of Sentences-Error Analysis, Vocabulary building. (10 hours)

Learning Outcomes:

At the end of the unit, the student will be able to:

- Use structures and tenses accurately
- apply the right verb to the right subject in a sentence
- Detect incorrect sentences in English and write their correct form
- Acquire new vocabulary and use in speaking and writing

UNIT - II

ORAL PRESENTATION: What is a Presentation? Types of Presentations, Technical Presentation – Paper Presentation, Effective Public Speaking, Video Conferencing. (8 hours)

Learning Outcomes:

At the end of the unit, the student will be able to:

- Overcome speaking anxiety prior to presentation
- Plan and structure effective presentations that deliver persuasive messages
- Prepare slides that can catch the attention of the audience
- Engage the audience
- Skills in organizing, phrasing, and expressing the ideas, opinions and knowledge.
- Facilitate and participate in a video conference effectively

UNIT III

DOCUMENTATION : Letter –Writing, E-mail Writing & Business Correspondence, Project Proposals, Report Writing, Memos, Agenda, Minutes, Circulars, Notices, Note Making. (10 hours)

Learning Outcomes:

At the end of the unit, the student will be able to:

- Write a business letter, which includes appropriate greetings, heading, closing and body and use of professional tone.
- Draft crisp and compelling emails

- Draft project proposals, reports and memos
- Prepare agenda and draft minutes
- Prepare circulars, notices and make notes.

UNIT IV

CREATIVE WRITING: Paragraph Writing, Essay writing, Dialogue Writing, Précis Writing, Expansion of Hints, Story Writing. (6 hours)

Learning Outcomes:

At the end of the unit, the student will be able to:

- Write paragraphs on familiar and academic topics using a topic sentence, supporting detail sentences and a conclusion sentence.
- Learn the structure of a five-paragraph essay and write essays that demonstrate unity, coherence and completeness
- Structure natural, lucid and spontaneous dialogues
- Draft clear, compact logical summary of a passage
- Recognize the elements of a short story and develop their functional writing skills.

UNIT V

PLACEMENT ORIENTATION: Resume preparation, group discussion – leadership skills, analytical skills, interviews –Types of Interviews, Preparation for the Interview, Interview Process. (8 hours)

Learning Outcomes:

At the end of the unit, the student will be able to:

- Write a professional resume that highlights skills, specific to the student's career field
- Acquire the personality traits and skills required to effectively participate in a G.D
- Understand the purpose of interviews
- Be aware of the processes involved in different types of interviews
- Know how to prepare for an interview
- Learn how to answer common interview questions

Text Books :

1. Essentials of Business Communication by Rajendra Pal and J S Korlahahi, Sultan Chand & Sons.
2. Advanced Communication Skills by V. Prasad, Atma Ram Publications.
3. Effective Communication by Ashraf Rizvi, McGraw Hill Education; 1st Edition , 2005.
4. Interviews and Group Discussions How to face them by T.S.Jain, Gupta, 1st Edition, Upkar Prakashan, 2010.
5. High School English Grammar and Composition by P.C.Wren & Martin, N.D.V.Prasada Rao S.Chand.

M.Sc. CHEMISTRY - II SEMESTER
SCY722: INORGANIC CHEMISTRY LAB

Hours per week: 9
Credits: 3

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

1. Inorganic Synthesis

Preparation of following complexes

- a) Tetraaminecopper(II) sulphate
- b) Potassium tris (oxalato) ferrate(III) trihydrate
- c) Potassium tris (oxalato) aluminate(III)
- d) Tris (thiourea) copper(I) sulphate
- e) Hexaaminecobalt(III) chloride
- f) Characterization of above complexes by Powder X-ray diffraction and FT-IR techniques

2. Determination of metal ions

- a) Zinc using potassium ferrocyanide
- b) Zinc using EDTA
- c) Magnesium using EDTA
- d) Cerium (IV) using potassium ferrocyanide
- e) Iron(III) by photochemical reduction method

3. Separation of ions using Ion Exchange Chromatography

- a) Zinc and Magnesium
- b) Chloride and Bromide

4. Synthesis of nanomaterials and determination of particle size distribution Using DLS (Diffraction Light Scattering) technique

Books:

- 1 Vogel's Qualitative Inorganic Analysis - VIIth Edition Revised by G. Svehla, Pearson Education Ltd., 1996.

M.Sc. CHEMISTRY - II SEMESTER
SCY724: COMPUTATIONAL CHEMISTRY LAB

Hours per week: 6

Credits: 2

Continuous Evaluation: 100 marks

CHEMDRAW:

Drawing the structures of simple aliphatic, aromatic, heterocyclic compounds with different substituents. Identification of IUPAC name

Computational Quantum Chemistry (CQC) Studies:

- Singlepoint energies using HF theory: water, formaldehyde and biphenyl
- Geometry optimizations and MO energies using HF theory: ethylene, butadiene and biphenyl; ionization potential and electron affinity
- Geometry optimization using DFT: water, methane, carbon tetrachloride, benzene and m-dinitrobenzene; dipole moments
- Frequency analysis using DFT: stable compound, transition state
- Modeling chemical reactions using DFT: keto-enol tautomerism of acetone and *syn-anti* isomerization of 1,3-butadiene

Text Books:

1. J. Foresman and A. Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
2. Hehre W. J., Shusterman A. J. and Huang W. W., A Laboratory Book of Computational Organic Chemistry', 1996.

M.Sc. CHEMISTRY (With specialization in Analytical Chemistry) - III SEMESTER
SAC801: CONCEPTS OF ANALYTICAL CHEMISTRY

Hours per week: 4
Credits: 4

Semester End Examinations: 60 Marks
Continuous Evaluation: 40 marks

Preamble: The students of postgraduate program in science need to be conversant with the various instrumental and analytical techniques in analytical chemistry for training graduate students as analytical chemists.

Course objective:

The concept of qualitative and quantitative methods in analytical chemistry will be introduced to graduate students specializing in analytical chemistry.

Students will also learn the fundamental concepts of various methods for quantitative analysis.

UNIT-I

Basic principles of volumetric analysis I: Expression of concentrations and Stoichiometric calculations. **Neutralization Titrations:** titration curves, Indicators, applications of neutralization titrations. **Non-aqueous solvent:** Characteristic of solvents, non-aqueous titrations- types of reactions, indicators and applications: i). Determination of acids, ii) Determination of bases, iii) Karl-Fischer reagent for the determination of moisture content in drugs and other samples

Learning outcome: The students will be familiar with the basic concepts of volumetric analysis. The students will also learn the titrimetric analysis in aqueous and non-aqueous medium. The students will be familiar with the various applications of non-aqueous titrations. The students will be taught about Karl fisher titration and applications.

UNIT-II:

Basic Principles of volumetric analysis II: Complexation Titrations: Types of titrations, EDTA titration curves, masking and de-masking agents. Detection of end point in EDTA titrations –metal ion indicators and applications of complexometric titrations. **Precipitation Titrations:** Law of mass action, solubility product, ionic product, principle, indicators for precipitation titrations Volhard method, Fajans method and Mohr's method. **Redox Titrations:** titration curves, redox indicators and applications of redox titrations

Learning Outcome: The students will be familiar with details of basic principle and applications of complexometric, redox and titrimetric procedures.

UNIT-III:

Electrochemical sensors and measurements: Measurement of pH- principle, glass membrane electrode, membrane potential, liquid junction potential and calibration. Measurement of potential: Formal Potential and factors affecting formal potential. potentiometric titrations. Ion-selective electrodes: principle, types and applications. Measurement of conductance: High frequency titrations-theory, instrumentation, applications, advantages and disadvantages of HF titrations.

Learning outcome: The students will be familiar with the details of the basic principle, instrumentation and pHmetric measurement. The students will also be taught the concept of direct potentiometric measurements using ion selective electrodes, their types and various applications in analytical measurements. The students will also learn the concept, instrumentation and applications of high frequency titrimetric measurements.

UNIT-IV

Introduction to gravimetric analysis: precipitation methods, the colloidal state, super saturation, nucleation and crystal growth. Solubility and particle size, completeness of precipitation, purity of precipitates, aging. Drying and ignition of precipitates, Precipitation from homogeneous solution (PFHS). **Principles of Electro-gravimetry:** Electro-gravimetric analysis: Principle, important terms in electro-gravimetry, -decomposition voltage or decomposition

potential, over volt-age and their importance, instrumentation, electrolysis at constant current, electrolysis at controlled potential, determination of Sb ,Cu, Pb, Sn in an alloy by controlled potential electrolysis.

Learning outcome: The students will learn the details of the concept of gravimetric analysis, detailed procedure, factors affecting gravimetric analysis n quality of precipitate. The students will also be familiar with the concept of precipitation from homogenous solution, applications and contrasts.

The students will also learn about the principle, instrumentation and applications of electro-gravimetry in analytical measurements.

UNIT-V

Coulometric Analysis: Principles of coulometric analysis with constant current, coulometric analysis with controlled potential, applications of coulometric methods -Determination of Ni and Co by controlled potential coulometric analysis, Determination of As (III) and Fe (II) by controlled current analysis.

Amperometric titrations – Theory, apparatus, types of titration curves, successive titrations and two indicator electrodes – applications. Technique of amperometric titrations with the dropping mercury electrode – Titration with the rotating platinum microelectrode.

Learning Outcome: The students will be familiar with the principle , instrumentation and applications of electroanalytical techniques of coulometry and amperometry.

Textbooks:

1. Quantitative Analysis, R.A.Day & A.L.Underwood, Prentice -Hall of India,1991
2. Chemical analysis - H.A. Laitinan, McGraw Hill Book Co.,1975
3. Analytical Chemistry An Introduction by D.A. Skoog, D.M. West and F.J. Holler, Sanders College Publishing, New York, 2004
4. Analytical Chemistry, Gary D Christian, John Wiley and Sons inc,2003.
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5. Volumetric Analysis, Vol. III -I. M. Kolthoff and R. Welcher, Interscience Public, New York,1969
6. Vogel's textbook of Inorganic Quantitative Analysis - J. Bassett et al. ELBS ,2005

Reference Books:

1. Quantitative Chemical Analysis – I.M. Kolthaff, E.B Sandal, Macmillan, Company, London, 1969.
2. Analytical chemistry for Technicians, John Kenkel, Lewis publishers, 3rd Edn, 2003

M.Sc. CHEMISTRY (Specialization in Organic Chemistry) - III SEMESTER
SOC801: ORGANIC SYNTHESIS

Hours per week: 4

Semester End Examination: 60 Marks

Credits: 4

Continuous Evaluation: 40 marks

The students pursuing this course would have to develop in depth understanding of various aspects of the subject. The conceptual understanding, development of experimental skills, designing and implementation of novel synthetic methods, developing the aptitude for academic and professional skills, acquiring basic concepts for structural elucidation with hyphenated techniques, understanding the fundamental biological processes and rationale towards computer assisted drug designing are among such important aspects.

Course Objectives:

- To learn C-C, C = C bond formation by various method reagents in organic synthesis.
- To learn the mechanism of condensation, oxidation and reduction. Synthetic application of reagents
- To learn the mechanism of addition and elimination reaction, oxidation of methylene to carbonyl, oxidation of aryl methanes, allylic oxidation of olefins, reduction and coupling reaction
- To learn about general consideration of molecular asymmetry and dissymmetry, configuration metals of determinations mechanisms of reactions and rearrangement.
- To introduce retrosynthetic analysis and modern synthetic reagents
- The objective of the course is to appraise the students about the organometallic Chemistry.
- Define Methodologies in organic synthesis and explain carbonyl compounds

SYLLABUS

Unit I:

Formation of carbon-carbon single bonds: Alkylations via enolate, enamine and related reactions, umplong (dipole inversion), carbon-carbon bond formation through organo lithium, organo palladium Heck reaction & Suzuki coupling.

Learning Outcomes

By the end of this Unit, the student will be able to

- To know synthetically the processes relevant organic-chemical reactions and be able to discuss the mechanism of these reactions
- To know about the stereo-chemical problems in relation to chemical transformations
- Identify the mechanism of selected name reactions
- Predict the basic mechanism of an organic reaction

Unit II :

Formation of carbon-carbon double bonds: Elimination reactions - pyrolytic, syn eliminations, sulphoxide-sulphinat rearrangement, Peterson reaction, Wittig reaction, alkenes form arylsulphonylhydrazones, Eschenmoser fragmentation, olefin metathesis (Grubbs reaction).

Learning Outcomes

By the end of this Unit, the student will be able to

- To know the detail study of wood-ward, provost hydroxylation, selenium dioxide, crown ethers and Peterson's synthesis and Wilkinson's catalyst.
- To know the various applications in named reactions.

Unit III:

Organoboranes: Preparation of Organoboranes, hydroboration, disiamyl borane, hexyl borane, 9-BBN and diisocamphenyl borane, functional group transformations of organoboranes-oxidation, protonolysis and rearrangements. Formation, of carbon - carbon-bonds viz organoboranes, carbonylation, the cyanoboration process and reaction of alkenyl boranes.

Organosilanes: Synthetic applications of trimethylsilyl chloride, dimethyl-t-butylsilyl chloride, trimethylsilyl cyanide, synthetic applications of- α silyl carbanion and β -silyl carbonium ions.

Learning Outcomes

By the end of this Unit, the student will be able to

- To learn about the synthesis and applications of the organic reagents like 9-Borabicyclo(3.3.1)nonane (9-BBN) and organosilanes
- Have insight into the use of modern methods to characterize organometallic compounds.

UNIT-IV

Reduction: Catalytic hydrogenation (homogeneous and heterogeneous), reduction by dissolving metals, reduction by hydride transfer reagents, complex metal hydrides, reduction with hydrazine and diamide,

Oxidation: Oxidations of hydrocarbons, alkenes, alcohols aldehydes and ketones oxidative coupling reactions. Use of $\text{Pb}(\text{OAc})_4$, NBS, CrO_3 , SeO_2 , MnO_2 , KMnO_4 , OsO_4 . Wood ward and Provost hydroxylation.

Learning Outcomes

By the end of this Unit, the student will be able to

- Predict the structure and mechanism of reactions involving selected oxidizing and reducing agents
- To acquire knowledge about the reagents which causes oxidation in various compounds
- To learn about the two types of reduction reactions like complete reduction and selective reduction

- Knowledge of the increasingly important role played by organic and transition metals reagents and catalysts with their corresponding proposed reaction mechanisms.

Unit V

Retrosynthesis the disconnection approach: Introduction, terminology, principles convergent and linear synthesis, One group C–X (X = hetero atom), C–C disconnections and two groups C–X and C–C disconnections with reference to 1,1; 1,2; 1,3; 1,4 and 1,5 difunctionalised compounds. Retrosynthesis and synthetic strategies with examples - salbutamol, benzocaine, paracetamol and dinocap.

Learning Outcomes

By the end of this Unit, the student will be able to

- Describe the important concepts of the organic chemistry for the synthesis of new molecule, introduction of different functional group.
- Formulate the chemistry of protection and de-protection strategies involved in hydroxyl group by ether and ester, carbonyl group, and amino groups.
- Analyze the chemistry of protection and de-protection strategies involved in hydroxyl group by ether and ester, carbonyl group, and amino groups and functional group interconversion by substitution reactions.
- Retrosynthetic approach to planning organic syntheses and Conversion of different functional group via rearrangement reaction

Suggested Text Books:

1. A Textbook of Organic Chemistry: Book by R.K. Bansal, SBN: 9788122420258 Publisher: New Age International Year of publishing: 2007.
2. Organic Reaction Mechanisms, Raj K. Bansal. New Age International Publishers, 4th Edn., New Delhi, 2015.
3. Agarwal, O.P. Unified Chemistry, Vol I, II, & III, Jai Prakashnath Publications, Fiftieth Edition, 2016.
4. Bahl, A & Bahl, B.S. *A text book of Organic Chemistry*, S. Chand & Company Pvt.Ltd. 2014.

Reference Books:

5. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
6. Kalsi, P. S. *Stereochemistry Conformation and Mechanism*, New Age International, 2005.
7. McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.
8. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

M.Sc. CHEMISTRY (With specialization in Analytical Chemistry)- III SEMESTER
SAC803: INSTRUMENTAL METHODS OF ANALYSIS

Hours per week: 4

Credits:4

Semester Examination: 60 Marks

Continuous Evaluation: 40 marks

Preamble:

The students of postgraduate program in Chemistry need to be conversant with the various instrumental method of analysis in chemistry. Therefore, It helps the student familiarize with the techniques essential for developing the foundation of Instrumental methods in analytical chemistry

Course Objective: The course aims to equip the students with the fundamental knowledge of the theory behind many techniques in analytical chemistry and their use in range of applications, as well as the limitations of the various techniques

UNIT I- Thermal methods of analysis: Thermo gravimetry-theory, instrumentation, applications with special reference to $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ and CaCO_3 . Basic idea of differential thermal analysis (DTA): principle and instrumentation. Difference between TGA and DTA. Differential scanning calorimetry: principle and instrumentation.

Learning outcome: Fundamental idea of various Thermo analytical techniques. Applications of the techniques.

UNIT II

Flame photometry: Theory and instrumentation. Analyses of Na, K, Ca, and Mg.

Atomic Absorption Spectrometer: Theory, instrumentation, chemical and spectral interferences, Applications

Induced couple plasma spectroscopy: Theory, Instrumentation and applications of ICP-OES

Learning outcome: The student learns optical method of spectroscopy for quantitative analysis. The difference and various applications of the optical methods.

UNIT III

Principles of chromatography: Classification of different chromatographic methods, adsorption and partition isotherms, column capacity, retardation factor, retention time and retention volume, gradient elution, height equivalent theoretical plate (HETP)

High performance liquid chromatography: Theory and instrumentation: pumps, column, detectors-UV detector, refractive index detector, Fluorescence detector, photo diode array detector and applications.

Gas liquid chromatography: Theory and instrumentation: columns (packed and capillary columns), detector: thermal conductivity detector, flame ionization detector, electron capture detector, nitrogen-phosphorus detector, photo ionization detector, and applications.

Learning outcome: Students will learn the fundamentals of chromatographic separation. The students will also learn the difference and instrumentation of Liquid and gas chromatographic separations.

UNIT-IV-Voltametry: Principle of polarography residual current, migration current, diffusion current, half-wave potential, Ilkovic equation.

Instrumentation: Dropping mercury electrode (DME), advantages and disadvantages of DME, qualitative and quantitative analysis of inorganic ions - Cu, Pb Cd and Zn.

Anode Stripping Voltametry: Principle and instrumentation. Hanging drop mercury electrode, application in the analysis of some selected metals.

Learning Outcome: Students will learn the fundamental and application of different electro-analytical techniques used for quantitative analysis.

UNIT V –

Mass Spectrometry: Basic principle, Instrumentation: methods of Ionization & mass analyzers and general applications.

X-ray Fluorescence Spectroscopy: X-ray spectrometers, energy dispersive and wavelength dispersive techniques, instrumentation, matrix effects and applications.

Learning Outcome: Students will learn the fundamental principle, instrumentation and application of X ray spectroscopy

Textbooks:

1. Instrumental methods of analysis - H.H. Willard, Meritt Jr. and J.A. Dean, CBS Publishers and distributors, 6th Edition, 1986.
2. Principles of instrumental analysis – Douglas A. Skoog, F. James Holler and R. Crouch, Cengage Learning, 6th edition, 2006.
3. Vogel's textbook of Quantitative Inorganic analysis - J. Basset, R.C. Denney, G.H. Jeffery and J. Mendham, Prentice Hall, 6th edition, 2000
4. Industrial methods of analysis - B.K.Sarma, Goel Publishing House, Meerut, 1997
5. Instrumental methods of Analysis – G.R. Chatwal and S. Anand, Himalaya publishing House, 13th reprint, 1999.
6. Analytical Chemistry – S.Usha Rani, Macmillan India Limited, 2001

Reference Books:

1. Instrumental methods of Analysis – Galen S. Ewing, McGraw Hill Higher Education, 5th edition, 1985
2. Handbook of Instrumental techniques for Analytical Chemistry, Frank Settle, Prentice Hall, 1997.

M.Sc. CHEMISTRY (Specialization in Organic Chemistry) - III SEMESTER
SOC803: ORGANIC SPECTROSCOPY

Hours per week: 4

Credits: 4

Semester End Examination: 60 Marks

Continuous Evaluation: 40 marks

Preamble

This course is designed to enable various spectroscopic technique, viz: To enable them the principles of IR, UV –Vis, NMR, Mass spectroscopy and their application to ascertain the structure of organic compounds

Course Objectives:

- To explain the principle of IR, various functional groups identification, factors affecting vibrational frequencies
- To explain laws of absorption in UV-Vis, presence of conjugation, chromophore/auxochrome / aromatic rings
- To explain principle of NMR, chemical shift, coupling constant, equivalence/nonequivalence of protons and carbons, anisotropy
- To explain Improved NMR techniques: chemical and instrumental techniques
- To explain principle of Mass spectroscopy, ionization methods, fragmentation technique

UNIT-I

Infrared spectroscopy: Basic theory, units of frequency wave length and wave number, molecular vibrations, functional group and fingerprint regions, fundamental vibrations and overtones, factors influencing vibrational frequencies, sampling techniques, characteristic frequencies of organic molecules and interpretation of spectra.

Learning Outcome

At the end of the unit, the student will be able to

- know the basic theory of IR
- functional group and fingerprint regions
- fundamental vibrations and overtones, calculations
- factors influencing vibrational frequencies, sampling techniques
- Characteristic frequencies of organic molecules and interpretation of spectra.
- identify the spectra of various compounds with the help of IR spectral patterns and values, then to assign the probable structure of unknown organic compounds

UNIT-II

Ultraviolet spectroscopy: Introduction- the absorption laws, measurement of the spectrum, chromophores, definitions; Woodward-Fieser rules for dienes, α,β -unsaturated carbonyl compounds and aromatic compounds; applications of UV spectroscopy to organic compounds. Optical rotatory dispersion and circular dichroism: Phenomena of ORD and CD. Classification of ORD and CD Curves.

Learning Outcome

At the end of the unit, the student will be able to:

- the absorption laws,
- measurement of the spectrum

- Calculation of λ_{max} values by Woodward-Fieser rules for dienes, α,β -unsaturated carbonyl compounds and aromatic compounds
- ORD and CD

UNIT-III

Nuclear magnetic resonance spectroscopy: Proton and Carbon ^{13}C NMR. The measurement of spectra - the chemical shift, equivalence and nonequivalence of protons, the intensity of NMR signals and integration. Factors affecting the chemical shifts, spin-spin coupling to ^{13}C - ^1H , ^1H - ^1H first order coupling, some simple ^1H - ^1H splitting patterns, the magnitude of ^1H - ^1H coupling constants.

Learning Outcome

At the end of the unit, the student will be able to:

- Principle of NMR, chemical shift, coupling constant
- Equivalence/nonequivalence of protons and carbons
- Factors affecting the chemical shifts
- assign the probable structure of unknown compounds

UNIT-IV

Improving the NMR spectrum: chemical techniques: deuteration, trifluoroacetylation, shift reagents, instrumental techniques: spin decoupling and spin tickling, INDOR, the Nuclear Over Hauser Effect. FT NMR spectroscopy, 2D-NMR (COSY & HETCOR)

Learning Outcome

At the end of the unit, the student will be able to:

- Improved NMR techniques: chemical and instrumental techniques
- INDOR, the Nuclear Over Hauser Effect.
- FT NMR spectroscopy
- 2D-NMR (COSY & HETCOR)

UNIT-V

Mass spectroscopy: Basic Principles, Isotope abundances, the molecular ion, metastable ions, nitrogen rule. Introduction to Ionisation techniques, fragmentation processes, and fragmentation associated with functional groups, rearrangement and mass spectra of some chemical classes.

Learning Outcome

At the end of the unit, the student will be able to:

- Principle of Mass spectroscopy
- ionization methods,
- fragmentation technique,
- mass spectra of some chemical classes

Text books:

1. Organic Spectroscopy, Jagmohan, Narosa Publications., 2004
2. Organic Spectroscopy, P.S .Kalsi, New-age International Publication, 2007
3. Organic Spectroscopy, Y.R.Sharma, S.Chand Publication, 2014
4. Introduction to Organic spectroscopy, Donald Pavia, G.Lampman, G,Kritz, J Vyvyan. Cengage Learning, 2007
5. Spectroscopy by H.Kaur, A Pragati Prakasan, 9th ed., 2014.
6. Spectroscopic Methods in Organic Chemistry. Forth Edition D.M. Williams and I. Fleming
Tata – Mc.Graw Hill, New Delhi, 1990.
7. Organic Spectroscopy: Principles, Problems and their solutions, Jagdamba Singh & Jaya Singh, Pragati Prakashan, First Edition, 2016.

Reference Books:

1. Spectrometric identification of Organic Compounds, Fourth Edition, R.M. Silverstein;

- C.Vasslellr and T.C. Merrill, John Wiley, 1974
2. Applications of absorption spectroscopy of Organic Compounds J.R.Dyer, Prentice Hall of India, New Delhi, 1984.
 3. Organic Spectroscopy, Second Edition, W.Kemp, ELBS Macmillan, 1987

M.Sc. CHEMISTRY(With specialization in Analytical Chemistry) - III SEMESTER
SAC805: QUALITY ASSURANCE AND QUALITY CONTROL

Hours per week: 4

Credits: 4

Semester End Examination: 60 Marks

Continuous Evaluation: 40 marks

Preamble: Quality management activities are those that ensure that a company's products are exactly what they are supposed to be, that is, they meet all their specifications. Quality assurance (QA) and quality control (QC) are two of the main activities that are required to ensure a quality product. QA is a set of activities that ensures that development and/or maintenance processes are adequate in order for a system to meet its objectives, whereas QC is a set of activities designed to evaluate the developed products. Another way to look at it would be to think of QA as preventing and detecting quality problems and QC as detecting errors in the product.

Course Objective: To make student familiar with pharmaceutical industry mainly confined to quality of drugs. maintenance of instruments and equipments used for doing laboratory experiments. To make students familiar with the quality objectives, Good laboratory practice by QMS.

UNIT- I

Characteristics of an analysis: Classification of errors, accuracy-absolute and comparative method, propagation of errors, precision, significant figures, mean and standard deviation, the confidence limit, Test of significance-Q-test, T-test and F-test, control charts, Quality of an analytical procedure.

Learning outcome: One should aware of factors responsible for deviation in the results. The detail description of the factors responsible to establish the procedure should be known

UNIT- II

Quality assurance and management systems: Elements of quality, quality control, quality assurance, Triple role concept, quality process model. Customer requirement of quality, quality assurance in design, development, Statistical process control, statistical quality control and acceptance sampling

Learning outcome: One should aware the terminology and models should be adopted to maintain the quality of the finished product.

UNIT-III

Quality and quality management system: Quality objectives-ISO standards concept: ISO9000, ISO14000 and its requirements.

Good laboratory practice (GLP) – Introduction, history of GLP, Principles of good manufacturing practice, basic issues of GLP, GLP status in India

Learning outcome: Significance of Quality objectives-ISO (ISO9000 &14000) and its requirements. Measures should be taken for Good laboratory practice (GLP) , good manufacturing practice and basic issues of GLP.

UNIT-IV

Calibration and maintenance of Instruments / Equipment: Instrument calibration – linear calibration curves, equipment calibration, frequency of calibration, calibration of common laboratory instrument and equipment

(Analytical balances, volumetric glassware, ovens, furnaces, UV / Visible spectrophotometer, pH meter, conductivity meter, IR spectrophotometer etc.,). Maintenance of instruments and equipment.

Validation of analytical method- methodology, -limit of detection, limit of quantification, range, sensitivity, selectivity and specificity, quality control-principles of Ruggedness/Robustness, Analytical method development, optimization and validation using HPLC for pharmaceutical dosage forms and bulk drugs and GC-MS for residual solvents.

Learning outcome: One should know the Calibration and maintenance of Instruments / Equipment: used for analysis of various materials. Student should also familiar with methodology adopted for validation of analytical method.

UNIT-V

General idea regarding pharmaceutical industry.- Introduction, Definition and classification of drugs, Quality of drugs, Sources of impurities in pharmaceutical chemicals and raw materials. Impurity profiling, classification of impurities, dissolution techniques of drugs, Significance of stability studies, types of stability studies, quantification of impurities. Basic concept of ICH guidelines for impurity profiling and stability studies.

Learning outcome: Familiar with classification of drugs, Quality of drugs, Sources of impurities in pharmaceutical chemicals and raw materials, Impurity profiling. Significance of stability studies, and basic concept of ICH guidelines for impurity profiling.

Textbooks:

1. Quality Assurance and Quality Management in Pharmaceutical Industry, Y. Anjaneyulu, R.Marayya, Pharma Book syndicate, 2002.
- 2 Analytical Chemistry, Gary D Christian, John Wiley and Sons Inc, 2003.

Reference Books:

1. Fundamentals of Analytical Chemistry, An Introduction, D.A. Skoog, D.M. West F.J. Holler and S R. Crouch, Sanders College Publishing, New York, 2004
2. K.V.S.G. Murali Krishna, An introduction ISO 9000, ISO 1400 Series, Environmental Management
3. Analytical Method Development and Validation, Michael Swartz & Swartz Swartz, CRC press.1997
4. Quality Assurance in Analytical Chemistry, Wenclawiak, M.Koch, Springer, Germany, 2006.

M.Sc. CHEMISTRY (Specialization in Organic Chemistry) - III SEMESTER
SOC805: PERICYCLIC REACTIONS AND PHOTOCHEMISTRY

Hours per week: 4

Semester End Examination: 60 Marks

Credits: 4

Continuous Evaluation: 40 marks

Preamble

This course is designed to enable the students aware about how an organic saturate or an unsaturated compound behave under different condition (Thermal or Photochemical). Stereochemistry of reactions, Pericyclic Reactions: FMO approach, various rules. Cycloadditions: Antarafacial and suprafacial additions; Sigmatropic Rearrangements, Organic Photochemistry, Photochemistry of unsaturated systems, Photochemistry of aromatic compounds. At the end, to make the organic reaction mechanism easy and handy to the student

Course Objectives

- To explain the Radical substitution Mechanism with some specific reactions
- To explain Pericyclic Reactions
- To explain Antarafacial and suprafacial cyclo-additions,
- To explain Sigmatropic rearrangements
- To explain Organic Photochemistry
- To explain Photochemistry of unsaturated systems and aromatic compounds

UNIT: I

Radical substitution Mechanism: Reaction at sp^3 carbon, reactivity in aliphatic substrates reactivity at bridged position, reactivity at sp^2 carbon. Reactivity in aromatic substrates, neighbouring group assistance in free radical reactions, effect of reactivity in the attacking radical, effect of solvent on reactivity, halogenation at an alkyl carbon and allylic carbon, hydroxylation at aromatic carbon by means of Fenton's reagent, oxidation of aldehydes to carboxylic acids, formation of cyclic ethers with $Pb(OAc)_4$ Reed reaction, Kolbe reaction and Hunsdiecker reaction.

Learning Outcome

At the end of the unit, the student will be able to

- reaction at sp^3 and sp^2 carbon. Reactivity in selective substrates
- effect of solvent on reactivity
- Fenton's reagent
- Reed, Kolbe and Hunsdiecker reaction.

UNIT: II

Pericyclic Reactions: Molecular orbital symmetry, frontier orbitals of ethylene, 1,3 Butadiene, 1,3,5-Hexatriene, allyl system, classification of pericyclic reactions FMO approach, Woodward-Hoffman correlation diagram method and perturbation of molecular orbital (Huckel-Mobius) approach for the explanation of pericyclic reactions under thermal and photo chemical conditions. Electrocyclic Reactions- Conrotatory and Disrotatory motions ($4n$) and ($4n+2$), allyl systems.

Learning Outcome

At the end of the unit, the student will be able to

- Molecular orbital symmetry, frontier orbitals of selected compounds
- classification of pericyclic reactions FMO approach
- pericyclic reactions under thermal and photo chemical conditions.
- Electrocyclic Reactions

UNIT: III

Cycloadditions: Antarafacial and suprafacial additions, notation of cycloadditions, $(4n)$ and $(4n+2)$ systems with a greater emphasis on $(2+2)$ and $(4+2)$ cycloadditions, explanation of cycloadditions with Woodward- Hoffman correlation diagram method and perturbation of molecular orbital (PMO) approach and chelotropic reactions.

Sigmatropic Rearrangements: FMO approach, and perturbation of molecular orbital (PMO) approach for the explanation of sigma tropic rearrangements under thermal and photochemical conditions, suprafacial and antarafacial shifts of H Sigmatropic shift involving carbon moieties, retention and inversion of configurations, $(1,3)$ $(3,3)$ and $(5,5)$ sigmatropic rearrangements detailed treatment of Claisen(Ireland-Claisen, Overman-Claisen, Jhonson-Claisen) and Cope rearrangements, fluxional tautomerism and aza-Cope rearrangement.

Learning Outcome

At the end of the unit, the student will be able to

- Antarafacial and suprafacial additions, notation of cycloadditions
- Woodward- Hoffman correlation diagram
- molecular orbital (PMO) approach and chelotropic reactions
- FMO approach, and PMO approach of sigma tropic rearrangements under thermal and photochemical conditions
- Sigmatropic rearrangements

UNIT: IV

Organic Photochemistry: Photochemical energy, Franck - Condon Principle, Jablonski diagram singlet and triplet states, dissipation of photochemical energy, photosensitization, quenching, quantum efficiency and quantum yield, experimental methods of photochemistry. Photochemistry of carbonyl compounds $n-\pi^*$ and $\pi-\pi^*$ transitions. Norrish type I and Norrish type II cleavages, Paterno-Buchi reaction. Photochemistry of enone – Hydrogen abstraction, rearrangement of α , β - unsaturated ketones and cyclohexadienes, photochemistry of p- Benzoquinones.

Learning Outcome

At the end of the unit, the student will be able to:

- Franck - Condon Principle,
- Jablonski diagram
- dissipation of photochemical energy
- Norrish type I and Norrish type II cleavages

UNIT – V

Photochemistry of unsaturated systems: Olefins, cis trans isomerisation and dimerisation, Photochemistry of 1,3 butadienes , photochemistry of cyclohexadienes. Photo oxidations and photo reductions.

Photochemistry of aromatic compounds – Excited state of benzene its 1, 2-1,3 1-4 additions, photo Fries rearrangements, photo Fries reactions of anilides, photosubstitution reactions of benzene derivatives. 1,3 and 1,4 alkyl shifts. Reactions of unactivated carbon-hydrogen bonds. The Hoffmann Löffler- Freytag reaction and the Barton reaction.

Learning Outcome

At the end of the unit, the student will be able to

- Photochemistry of unsaturated systems selected systems
- Photochemistry of aromatic compounds
- Reactions of unactivated carbon-hydrogen bonds

Text books:

1. Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, Mc. Graw Hill and Kogakush., 2006
2. Pericyclic reactions by S.N. Mukhrjee, Mcmilan., 2010
3. Molecular reactions and Photochemistry by Charles Dupey and O. Chapman, Prentice Hall, 2014

Reference Books:

1. The modern structural theory in Organic Chemistry by L.N. Ferguson, Prentice Hall, 1969.
2. Advanced Organic Chemistry, F.A.Carey and R-J Sundberg, Springer, 2007

M.Sc. CHEMISTRY - III SEMESTER

SCY841: GREEN CHEMISTRY

Hours per week: 4

Credits: 4

Semester End Examination: 60 Marks

Continuous Evaluation: 40 marks

Preamble: The students of postgraduate program in science need to be conversant with the various green techniques in synthetic and analytical chemistry. This course will lay the foundation for the student to be able to appreciate eco-friendly methods in chemistry and develop as a responsible chemist for the benefit of the society and environment.

Course objective:

The concept of green chemistry encompassing green chemistry strategies, concepts and practices will be introduced to the undergraduate students.

Students will also learn the fundamental concepts of various green synthetic methods and techniques for quantitative analysis.

The student will also learn Green separation and extraction for sample preparation

UNIT I: Introduction to Green Chemistry

Green chemistry - Introduction - need for green chemistry - goals of green chemistry - Anastas' twelve principles of green chemistry - Designing a green synthesis (tools) - choice of starting materials, solvents, catalysts, reagents, processes with suitable examples.

Learning outcome: The students will learn the goals and principles of green chemistry.

UNIT 2: Ionic liquids - synthesis, physical properties of ionic liquids - applications in alkylation, epoxidation, Friedel-Crafts reaction - Diels-Alder reactions - Knoevenagel condensations and Wittig reactions.

Phase Transfer Catalyst (PTC) - Definition - advantages, types of PTC reactions - synthesis of PTC, applications of PTC in organic synthesis - Michael reaction - alkylation of aldehydes and ketones. Wittig, generation of dihalocarbene, elimination reaction

Learning Outcome: The students will learn the properties of ionic liquids and synthesis of molecules using the green solvents- ionic liquids.

UNIT 3: Supercritical CO₂ - phase diagram - uses in extracting natural products, dry cleaning, bromination, Kolbe-Schmidt synthesis - Friedel-Crafts reaction. Dimethyl carbonate as a methylating agent in green synthesis.

Learning Outcome: The students will learn the modern extraction using CO₂ and applications of methylating agents for green synthesis

UNIT 4: Microwave and Ultrasound Assisted Reactions

Microwave activation - advantages of microwave exposure - Microwave assisted reactions, condensation reactions - oxidation, reduction reactions, multicomponent reactions.

Sonochemistry - use of ultrasound in organic synthesis (alternate source of energy) - saponification - substitution, addition, oxidation reactions, reductions.

Learning outcome: The students will learn the basic principle of microwave and sonication methods. Application of these green techniques for synthesis of compounds. Advantages and contrasts of the green methods versus conventional synthesis methods.

UNIT 5: Green Analytical Techniques

Micelle mediated extraction- Cloud point extraction and adsorptive micellar flocculation methods. Solid Phase Micro Extraction (SPME)

Learning outcome: The students will learn the details of instrumentation, application and contrasts of modern extraction methods

Text books:

1. "Green Chemistry", Paul T. Anastas and John C. Warner, Oxford University Press, Indian Edition, 2008.
2. New Trends in Chemistry", V. K. Ahluwalia and M. Kidwai, "Anamaya Publishers, 2nd Edition, 2007.
3. "An Introduction to Green Chemistry", V. Kumar, Vishal Publishers, 1st Edition, 2007.
4. "Green Solvents", V. K. Ahluwalia and R. S. Varma, Narosa Publishing, 1st Edition, 2009.
5. "Organic Synthetic Special Techniques", V.K.Ahluwalia and Renu Aggarwal, Narosa, 2nd Edition, 2009.
6. "Green Chemistry - Environmentally Benign Reactions", V. K. Ahluwalia, Ane books, India, 2006.

M.Sc. CHEMISTRY - III SEMESTER
SCY843: CHEMISTRY OF NANOMATERIALS

Hours per week: 4

Semester End Examination: 60 Marks

Credits: 4

Continuous Evaluation: 40 marks

UNIT-I

Introduction to Nanomaterials- Size Effects - difference between bulk and Nanomaterials - Definition of Nanomaterial - Classification Nanomaterials: Nanoparticles, Nanocrystal, 0-D Quantum dots, Nanostructured material (1-D Wire and rods, 2-D thin film, 3-D structures) - Carbon nanotubes (CNTs) : Single walled carbon nanotubes (SWNTs), Multiwalled carbon nanotubes (MWNTs) - Graphene. Influence of Nano structuring on mechanical (Abrasion and wear resistance, Super elasticity, Nanotribology), optical, electronic, magnetic and chemical properties.

UNIT-II

Synthesis and Characterisation of Nanomaterials: Synthesis of Nanomaterials: Bottom Up and Top Down Approach - Gas Phase synthesis of Nanomaterials - Wet chemical synthesis - Chemical Vapour Deposition (CVD). Characterisation of nanomaterials using UV-Visible Spectroscopy, Fluorescence Spectroscopy, Powder XRD, Particle size analysis by Dynamic Light Scattering (DLS), SEM, TEM, AFM techniques.

UNIT-III

Electronic and Photonic Molecular Nanomaterials: Optical luminescence and fluorescence from direct, band gap semiconductor nanoparticles - White LEDs - LEDs based on nanowires - LEDs based on nanotubes- LEDs based on nanorods - High Efficiency Materials for OLEDs - High Efficiency Materials for OLEDs.

UNIT-IV

Renewable Energy Technology: Energy challenges, development and implementation of renewable energy technologies - nanotechnology enabled renewable energy technologies – Nanomaterials and devices for energy transport, conversion and storage.

UNIT-V

Nanomaterials in Medicine: Introduction to Nanocarriers, Interactions of nanocarriers with blood stream, cellular targeting, Biological and chemical reagents for cell-specific targeting. Biodistribution of liposomes, dendrimers and Nanoparticles, Toxicity of nanocarriers, drug delivery, tissue regeneration, cancer detection, Luminescent nanoparticle probes for bio-imaging and diagnostics.

Text Books:

1. Textbook of Nanoscience and Nanotechnology, B.S. Murty, Universities Press, 2011
2. Nanochemistry: A chemical approach to Nanomaterials, Ozin Geoffrey A. and Andre C. Arsenault, Royal Society of Chemistry Publication, 2005.
3. Nano: The Essentials”, T. Pradeep, Tata McGraw Hill, 2007
3. Renewable Energy Resources, J. Twidell and T. Weir, E & F N Spon Ltd, 1986.

M.Sc. CHEMISTRY(With specialization in Analytical Chemistry) - III SEMESTER
SAC821: ELECTROANALYTICAL TECHNIQUES LAB

Hours per week: 9

Semester End Examination: 60 Marks

Credits: 3

Continuous Evaluation: 40 marks

Conductometry

1. Determination of weak acid and weak base
2. Determination of chloride using silver nitrate
3. Determination of mixture of NaOH and NH_4OH using HCl
4. Determination of Borax

PH metry

1. Determination of strength of commercial phosphoric acid by pH-metric titration.
2. Determination of Sodium carbonate by pH metric titration using HCl.
3. Determination of the strength of acetic acid, chloro-acetic acid and tri-chloroacetic acid by pH-metry using standard solution of NaOH.

Potentiometry

1. Determination of V (V) with Fe (II) using potentiometric end point.
2. Determination of Mn (VII) with Fe (II) using potentiometric end point.
3. Determination of Ce (IV) with Fe (II) using potentiometric end point.
4. Determination of a mixture of Ce (IV) and V (V) with Fe (II) using potentiometric End point.
5. Determination of a mixture of Mn (VII) and V (V) with Fe (II) using potentiometric end point.
6. Determination of Assay of Benzoic acid/oxalic acid by titrating with NaOH solution potentiometrically

Demonstration Experiments

1. Oxidation of Ferrocene and reduction of $\text{K}_3[\text{Fe}(\text{CN})_6]$ by Cyclic Voltammetry.

M.Sc. CHEMISTRY (With specialization in Analytical Chemistry)- III SEMESTER

SCY821: CHROMATOGRAPHIC SEPARATION and SPECTROSCOPY LAB -

Hours per week: 6

Semester End Examination: 60 Marks

Credits: 2

Continuous Evaluation: 40 marks

a) Separation and purification of inorganics and organic compounds by thin layer chromatography.

(b) Identification of functional groups by using IR and UV spectroscopy

(C) Interpretation of given NMR spectra and identification of organic Compounds

Text Books:

1. Text book of Practical Organic Chemistry, by Vogel, Pearson, 1978
2. Text book of Practical Organic Chemistry, by Mann and Saunders, Pearson, 2009

M.Sc. CHEMISTRY (Specialization in Organic Chemistry) - III SEMESTER
SOC821: MULTISTAGE SYNTHESIS LAB

Hours per week: 9
Credits: 3

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Multistage organic synthesis: Synthesis and purification of about six organic compounds involving three or more stages.

Text Books:

1. Text book of Practical Organic Chemistry, by Vogel, Pearson, 1978
2. Text book of Practical Organic Chemistry, by Mann and Saunders, Pearson, 2009

M.Sc. CHEMISTRY (Specialization in Organic Chemistry) - III SEMESTER
SCY821: CHROMATOGRAPHIC SEPARATION and SPECTROSCOPY LAB -1

Hours per week: 6
Credits: 2

Semester End Examination: 60 Marks
Evaluation: 40 marks

Continuous

a) Separation and purification of inorganics and organic compounds by thin layer chromatography.

(b) Identification of functional groups by using IR and UV spectroscopy

(c) Interpretation of given NMR spectra and identification of organic Compounds

Text Books:

1. Text book of Practical Organic Chemistry, by Vogel, Pearson, 1978
2. Text book of Practical Organic Chemistry, by Mann and Saunders, Pearson, 2009

M.Sc. CHEMISTRY(With specialization in Analytical Chemistry) - IV SEMESTER
SAC802: SEPARATION METHODS OF ANALYSIS

Hours per week: 4
Credits: 4

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Course Objective: The course aims to equip the students with the fundamental knowledge of the principle and instrumentation of separation techniques in analytical chemistry and their use in several of applications as well as the limitations of the techniques employed.

UNIT I

Solvent Extraction: Principle and processes of solvent extraction: distribution Law, different types of solvent extraction systems - batch extraction, continuous extraction and counter current extraction. Solvent extraction systems: Ion association systems and metal chelates. Basic principles of solid phase extraction, supercritical fluid extraction and Soxhlet extraction.

Learning outcome: Fundamental idea of liquid - liquid extraction. Idea about conventional and modern methods of extraction. Different solvent extraction systems and their applications in analytical chemistry

UNIT II

Planar chromatography: Thin layer chromatography: principle, chromatographic media-coating materials, activation of adsorbent, development of chromatographic plate and visualization methods- applications. HPTLC - Principle and technique.

Learning Outcome : The student learns the fundamentals of chromatographic separation principle, classification and important terms associated with the technique.

The students will also learn the principle of planar method of chromatographic separation, methodology and chromatographic media.

The students will also learn about similarities and contrasts of thin layer chromatography and the modern HPTLC method.

UNIT III

Principle, chromatographic media and applications: Gel Exclusion chromatography, Affinity Chromatography, Ion exchange Chromatography and Ion Chromatography.

Learning Outcome: Students will learn the fundamentals of different modes of high performance liquid chromatographic separation. The students will also learn details of instrumentation, mechanism and application of different modes of separation

UNIT IV

Capillary Electrophoresis: Principle - factors affecting ionic migration- effect of temperature, pH and ionic strength, electro-osmosis and supporting medium, Instrumentation. Modes: polyacrylamide gel electrophoresis, capillary zone electrophoresis, micellar electrokinetic electrophoresis, capillary gel electrophoresis and isoelectric focusing. Applications of capillary electrophoresis.

Learning Outcome: The Students will learn the fundamental principle, factors affecting separation and instrumentation of capillary Electrophoresis. The students will also learn the mechanism of separation in capillary electrophoresis apart from the applications of the technique application for quantitative analysis.

UNIT-V

Elementary Idea of Hyphenated Techniques: Theory, interfaces in hyphenation of the technique and applications of the following:

LC –MS, GC –MS, CE-MS

Learning Outcome: Students will learn the hyphenation of separation method with spectroscopic method for quantitative analysis. The students will learn the details of different inter-phases used for hyphenation of various separation techniques with mass spectroscopy.

Textbooks:

1. Separation methods, M.N. Sastri, Himalaya Publishing Company, Mumbai, 2005.
2. Chemical separation methods, John A Dean, Von Nostrand Reinhold, New York, 1969.
3. Analytical Chemistry – S. Usha Rani, Macmillan India Limited, 2001.
4. Principles and practice of Analytical Chemistry-F.W. Fifield and D. Kealey, Blackwell Science, First Indian reprint, 2004.
5. Separation Chemistry- R.P. Buddhiraja, New age international (P) Ltd. Publishers, 2nd edition, 2010.

Reference Books:

1. Chromatography concepts and contrasts – J.M. Miller, Wiley Interscience, 2nd edition, 2009.
2. Techniques and practice of Chromatography, R.P.W. Scott, Marcel Dekker Inc., New York, 1995.

M.Sc. CHEMISTRY(Specialization in Organic Chemistry) - IV SEMESTER

SOC802: CHEMISTRY OF NATURAL PRODUCTS

Hours per week: 4

Semester End Examination: 60 Marks

Credits: 4

Continuous Evaluation: 40 marks

Preamble

This course is designed to explain the students the isolation, structural elucidation, synthesis of the biologically active Microbial metabolites and shikimates; Terpenoids, Steroids, Alkaloids, Nucleic acids

Course Objectives

- To explain the isolation, structural elucidation, synthesis of the biologically active Microbial metabolites and shikimates
- To explain the isolation, structural elucidation, synthesis of the biologically active Terpenoids
- To explain the isolation, structural elucidation, synthesis of the biologically active Steroids
- To explain the isolation, structural elucidation, synthesis of the biologically active Alkaloids
- To explain the isolation, structural elucidation, synthesis of the Nucleic acids

UNIT-I

Study of isolation, structural elucidation, synthesis of the biologically active Microbial metabolites and shikimates : Pencillin G, Cephalosporin-C, Prostaglandin 15 (R) PGA2, Podophylotoxin and Etoposide; biosynthesis of Prostaglandin

Learning Outcome

At the end of the unit, the student will be able to understand:

- Isolation, structural elucidation, synthesis of Pencillin G, Cephalosporin-C, Prostaglandin 15 (R) PGA2, Podophylotoxin and Etoposide;
- biosynthesis of Prostaglandin

UNIT-II

Study of isolation, structural elucidation, synthesis of the biologically active Terpenoids: Forskolin, Taxol, Azadirachtin, and Santonin ; stereochemistry and biosynthesis of Santonin

Learning Outcome

At the end of the unit, the student will be able to

- Isolation, structural elucidation, synthesis of Forskolin, Taxol, Azadirachtin, and Santonin
- stereochemistry and biosynthesis of Santonin

UNIT - III

Study of isolation, structural elucidation, synthesis of biologically active Steroids: Cholesterol, Progesterone, Testosterone and Esterone ; stereochemistry and biosynthesis of Cholesterol

Learning Outcome

At the end of the unit, the student will be able to

- Isolation, structural elucidation, synthesis of Cholesterol, Progesterone, Testosterone and Esterone
- stereochemistry and biosynthesis of Cholesterol

UNIT -IV

Study of isolation, structural elucidation, synthesis, of biologically active Alkaloids: Morphine, Reserpine, Camptothecin and Strychnine; stereochemistry and biosynthesis of Morphine

Learning Outcome

At the end of the unit, the student will be able to

- Isolation, structural elucidation, synthesis of Morphine, Reserpine, Camptothecin and Strychnine
- stereochemistry and biosynthesis of Morphine

UNIT -V

Study of isolation, structural elucidation, synthesis of the Nucleic acids: Basic concepts of the structures of RNA and DNA and their hydrolysis products- nucleotides, nucleosides and heterocyclic bases; biosynthesis of pyrimidine and purine bases

Learning Outcome

At the end of the unit, the student will be able to

- Basic concepts of the structures of RNA and DNA and their hydrolysis products- nucleotides, nucleosides and heterocyclic bases
- biosynthesis of pyrimidine and purine bases

Text Books:

1. Organic Chemistry, Volume 2, Stereochemistry and chemistry of Natural products, I.L. Finar, 5th Edition, ELBS, 2002
2. Chemistry of Organic Natural Products; Vol & Vol II, Krishna Prakashan Media (P) Ltd, 43rd Edition, 2015
3. Chemistry of Natural Products: A Unified Approach, N.R. Krishnaswamy, University Press (India) Ltd., Orient Longman Limited, Hyderabad, 1999.

Reference Books:

1. Introduction to Organic Chemistry, A Streitweiser, CH Heathcock and E.M/ Kosover IV Edition, Mc.Milan, 1992
2. Chemical Aspects of Biosynthesis, John Mann, Oxford University Press, Oxford, 1996

M.Sc. CHEMISTRY(With specialization in Analytical Chemistry) - IV SEMESTER SAC842: ANALYSIS OF ORES, ALLOYS AND OTHER MATERIALS

Hours per week: 4

Semester End Examination: 60 Marks

Credits: 4

Continuous Evaluation: 40 marks

UNIT-I

Methods of dissolution and decomposition: Introduction, Scope of metallurgical analysis - General methods of dissolution of complex materials. Decomposition techniques in analysis: Principles of decomposition and dissolution, difference between decomposition and dissolution. Decomposition of samples with acids-HCl, HF, HNO₃, H₂SO₄, and HClO₄, Decomposition of samples by fluxes - alkali fusion -Na₂CO₃, NaOH, Acidic Fusion - Sodium hydro sulphate, Sodium pyro sulphate and sodium peroxide Sintering, difference between fusion and sintering, sintering with alkali carbonates .

UNIT-II

Analysis of ores and finished products

- (a) Iron ore - Analysis of the Constituents: Moisture, loss on ignition, total iron, ferrous iron, ferric iron, alumina, silica, lime, magnesia, Sulphur, Phosphorus, Manganese.
- (b) Manganese Ore - Analysis of the Constituents: Total manganese, MnO₂, SiO₂, BaO, Fe₂O₃, Al₂O₃, CaO, P and S.
- (c) Chromite Ore - Analysis of the Constituents - Chromium, SiO₂, FeO, Al₂O₃, CaO, & MgO
- (d) Aluminum Ore (Bauxite) - Analysis of the Constituents - Silica, Alumina, Fe₂O₃, Titania, P₂O₅, CaO, MgO.

UNIT III

Analysis of non-ferrous alloys.

Analysis of non-ferrous alloys: Introduction

- (i) Brass - Analysis of the constituents - Cu, Zn, Sn, Pb
- (ii) Bronze - Analysis of the constituents - Cu, Sn, Zn, Pb and Fe.
- (iii) Solder - Analysis of the constituents – Sn, Pb and Sb

UNIT-IV

Analysis of Ferro alloys and Finished products: Introduction

- (i) Ferro silicon - Analysis of the constituents – Si, C, P, S
- (ii) Ferro vanadium - Analysis of the constituents – V, C, P, S, Si
- (iii) Ferro manganese - Analysis of the constituents – Mn, S, C, P, Si
- (iv) Ferro chromium - Analysis of the constituents – Cr, C, Si

Analysis of steel

Analysis of steel for C, Si, S, P, Mn, Ni and Cr

UNIT V

Analysis of Coal, Cement, and fluxes:

- (a) Coal analysis –proximate and ultimate analysis.
- (b) Chemical Analysis of cement-silica, ferric oxide, alumina, lime, magnesia. Sulphide Sulphur (H_2S/S), K_2O , Na_2O , loss on ignition
- (c) Analysis of fluxes & Slag- limestone and dolomite, Blast furnace slag

Text books:

1. Technical methods of analysis-Griffin, McGraw Hill Book, 1927
2. Text book of Metallurgical analysis, B.C. Agarwal and S.P. Jain, Khanna publishers, 2003

Reference books:

- (a) Standard methods of chemical analysis, 6th edition, N. Howell Furman, D. Van Nostard Company Inc, Princeton, 1962
- (b) Commercial methods of analysis, Foster Dee Snell and Frank M Griffin, McGraw Hill, 1982
- (c) Decomposition Techniques in Inorganic Analysis - J. Dolezal, P. Povondra, Sulcek, 1979.
- (d) Standard methods of chemical analysis, F.J. Welcher, Van Nostrand Reinhold co, American Elsevier Publishing Company 1939

M.Sc. CHEMISTRY (Specialization in Organic Chemistry) - IV SEMESTER
SOC842: BIOORGANIC CHEMISTRY

Hours per week: 4

Credits: 4

Semester End Examination: 60 Marks

Continuous Evaluation: 40 marks

Preamble

This course is designed to introduce the students about the Bioorganic chemistry, Enzyme chemistry, Enzymes in synthetic organic chemistry, Enzymes and cofactors, Chemistry of amino acid and peptide bonds & Merrifield solid phase synthesis

Course Objectives

- To introduce Bioorganic chemistry, supramolecular chemistry, molecular recognition and drug design
- To explain mechanism of enzymes, enzyme catalysis
- To explain enzyme-catalyzed reactions and Co-enzyme chemistry
- To explain bioorganic chemistry of amino acid
- To explain the chemistry of peptide bond

UNIT-I: Introduction Bioorganic chemistry: Basic consideration, proximity effects in organic chemistry, molecular adaptation, supramolecular chemistry. Chemical mutation, Molecular recognition and drug design. Molecular asymmetry and prochirality.

Learning Outcome

At the end of the unit, the student will be able to:

- Basic concept, proximity, molecular adaptation, supramolecular chemistry.
- Chemical mutation, Molecular recognition and drug design.
- Molecular asymmetry and prochirality.

UNIT – II: Enzyme: General Characteristics of enzymes, specificity of enzymes, nomenclature and classification of enzymes, Mechanism of enzyme catalysis, factors influencing rate of enzymic reactions.

Mechanisms of enzyme action: Transition state theory, examples of typical enzyme mechanisms- chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

Application of Enzymes in synthetic organic chemistry.

Learning Outcome

At the end of the unit, the student will be able to know:

- enzymes, mechanism of enzyme catalysis,
- factors influencing rate of enzymic reactions
- mechanisms of enzyme action
- application of enzymes in organic chemistry

UNIT-III: Enzyme and Co-Enzyme chemistry: Enzyme-catalyzed addition, elimination, condensation, carboxylation and decarboxylation, isomerisation reactions.

Structure, biochemical functions and chemical reactions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD⁺, NADP⁺, FMN, FAD, lipoic acid and Vitamin B12.

Learning Outcome

At the end of the unit, the student will be able to understand:

- Enzyme-catalyzed addition, elimination, condensation reactions
- Structure and chemical reactions of coenzyme

UNIT – IV: Bioorganic Chemistry of amino acid: Analogy between organic reactions and biochemical transformations. Asymmetric synthesis of α – amino acids, asymmetric synthesis with chiral organometallic catalysts, Transition state analogues. Host-Guest complexation chemistry, antibodies as enzymes and crown ether chemistry.

Learning Outcome

At the end of the unit, the student will be able to know:

- Analogy between organic reactions and biochemical transformations.
- Asymmetric synthesis of α – amino acids
- Host-Guest complexation chemistry
- Crown ether chemistry

UNIT-V: Chemistry of peptide bond: Peptide synthesis, carboxyl protecting groups, amino protecting groups, Nonribosomal peptide bond formation, Peptide bond formation using DCC, synthesis of peptides by Merrifield solid phase synthesis. Chemistry of oxytocin and dolastatin.

Learning Outcome

At the end of the unit, the student will be able to know:

- Peptide synthesis
carboxyl protecting groups,
- amino protecting groups
- Merrifield solid phase synthesis
- Chemistry of oxytocin and dolastatin

Text Books:

1. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C.Penny, Springer-Verlag., 2010
2. Bioorganic Chemistry; Harish K. Chopra, Anupama Parmar, Parmjit S. Panesar:Narosa Publishing House, 2013
3. Bioorganic, Bioinorganic and Supramolecular Chemistry by J.P.Kalsi, P.S.Kalasi, New Age India Ltd, 2012

Reference Books:

1. Enzyme chemistry: Impact and Applications, Ed.Collin J Suckling, Chapman and Hall., 1990
2. Enzyme Mechanisms Ed, M.I.Page and A.Williams,Royal Society of Chemistry,1987
3. Fundamentals of Enzymology, N.C.Price and L.Stevens, Oxford University Press.,1999
4. Enzyme Structure and Mechanism, A Fershyt, W.H.Freeman.,1977
5. Biochemistry: The Chemical Reactions of Living Cells, D.E.Metzler, Academic Press, 2012

Hours per week: 4
Credits: 4

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

UNIT-I: Source of Impurities in Pharmaceutical Raw Materials and Finished Products: Raw materials, methods of manufacture, contamination-atmospheric, particulate, cross contamination, microbiological, process errors, packing errors, chemical instability, container contamination physical changes, temperature effects - Impurity profiling, classification of impurities. Dissolution techniques of drugs, Significance of stability studies degradation products, acid degradation, base degradation, peroxide degradation, and thermal degradation.

Functional group analysis: Classification of functional groups with suitable examples.
Determination of:

- 1) Functional groups imparting acidic nature – thiol, enediol, phenolic hydroxyl.
- 2) Functional groups imparting basic nature – Aliphatic and Aromatic primary, secondary and tertiary amines
- 3) Functional groups which impart neither acidic nor basic nature – Aldehydes, Ketones, Nitro, Methoxy.

Test and assay of raw materials and finished products:

Limit test, Characteristics of limit tests- specificity sensitivity, control of personal errors, loss on drying (NaCl), loss on ignition (ZnO),limit test for lead, arsenic chloride and sulphate, moisture determination by Karl fisher titration method.

Disintegration tests (tablets, capsules, pessaries and suppositories), dissolution tests-tablets, capsules

Analysis of drugs

Antibiotics – Chloramphenicol, and Tetracycline (Antibiotics)

Analgesic &Antipyretic – Asprin

Hypertensive -Methyldopa

Vitamins – Thiamine (B1) and ascorbic acid (C)

Steroids – Testosterone.

Role of FDA in pharmaceutical industry

Drug cosmetic act Definitions Drug, adulterated and spurious drugs, new drug cosmetics , Manner of labeling, GMP in brief (Schedule M), FDA. Role of FDA, introduction to new drugs, brief summary of different phases of test and approval for formulation of a drug.

- 1 Practical Pharmaceutical chemistry, 3rd edition, Volume 1, A.H.Beckett & J.B.Stenlake, Wiley, 1975.
- 2 Pharmaceutical analysis, T.Higuchi, CBS publishers, 2000.
- 3 Quantative organic analysis via Functional groups, Sidney Siggia, Wiley, 4th edn, 1979.
- 4 Pharmaceutical analysis, Ashitosh Kaur, New-age International, 2007.
- 5 Pharmaceutical Chemical Analysis, Ole Pedersen, CRC press, 2006.

M.Sc. CHEMISTRY (Specialization in Organic Chemistry) - IV SEMESTER
SOC844: MEDICINAL CHEMISTRY

Hours per week: 4

Credits: 4

Semester End Examination: 60 Marks

Continuous Evaluation: 40 marks

Preamble

*This course is designed to introduce the students about **Drug discovery and design, Drug structure and biological activity, Vitamines, Chemistry of selected drugs: Anticancer, Antimalarials, Anti-inflammatory, Sedatives, Antiulcers and antacids, Antiviral, Antihistaminic, Antiasthmatic agents***

Course Objectives

- To explain the lead Drug discovery and Design
- To explain the Drug structure and biological activity
- To explain the structure, physiological role and uses of Vitamins
- To explain some Anticancer, Antimalarials, Anti-inflammatory, Sedatives agents
- To explain some Antiulcers and antacids, Antiviral, Antihistaminic. Antiasthmatic agents

UNIT-I

Drug discovery and design: Lead discovery and lead modification, structure modification to increase bioavailability, lipophilicity, relationship between chemical structure and biological activity (SAR), QSAR- basic Concepts. Basic reactions of drug molecule synthesis.

Learning Outcome

At the end of the unit, the student will be able to know about lead discovery and lead modification for SAR & QSAR for biological activity

UNIT-II

Drug structure and biological activity: Pharmaceutically important functional groups-alcohols, carboxylic acid, amines, sulfonamides and carbonyl compounds. Chemistry of drug metabolism-absorption distribution, drug metabolism and excretion site specificity, stability, prolong release, minimum toxicity, patient acceptance.

Learning Outcome

At the end of the unit, the student will be able to know the importance of functional groups in drug, metabolism- absorption distribution and patient acceptance

UNIT-III

Vitamines : Structure, physiological role and uses of Vitamins A ,Vitamin D Thiamine (B1) and Pyridoxine (B6).

Learning Outcome

At the end of the unit, the student will be able to know the structure & uses of Vitamines

Chemistry of selected drugs- Synthesis and basic concept of action for the following drugs

UNIT-IV

(i) Anticancer: 5-Fluorouracil, Vincristine (ii) Antimalarials :Chloroquine , Chloroguanide (iii) Anti-inflammatory: Ibuprofen, Diclofenac Sodium (iv)Sedatives: Phenobarbital, Lidocaina.

Learning Outcome

At the end of the unit, the student will be able to know the chemistry of selected drugs and their mode of action

UNIT-V

(i) Antiulcers and antacids: Omeprazole, Ranitidine (ii) Antiviral: Acyclovir (iii) Antihistaminic: Terfenadine, Cinnarizine (iv) Antiasthmatic agents : Salbutamol and Beclomethasone dipropionate

Learning Outcome

At the end of the unit, the student will be able to know the chemistry of selected drugs and their mode of action.

Text Books

1. Medicinal Chemistry, A. Burger, Vol. I-III, Wiley Interscience Publications, New York, 1995.
2. Principles of Medicinal Chemistry, W. O. Foye, 3rd Edition, , Lea & Febiger/ Varghese Publishing House, Bombay, 1989
4. Medicinal Chemistry, A. Kar, Wiley Eastern Ltd., New Delhi, 1993.
5. The Organic Chemistry of Drug design and Drug action, Richard B. Silverman; II Ed.; Elsevier Acadmic Press, 2004
6. Medicinal Chemistry; Rama Rao Nadendla; PharmaMed Press, 2013
7. The Chemistry of Organic Medicinal Products; Glenn L.Jenkins,Walter H. Hartung,Kenneth E.Hamlin Jr.,John B.Data;IV Ed.; PharmaMed Press, 2010
8. Synthetic Drugs, G R Chatwal; Himalaya Publication, 1997

Reference book

1. Essentials of Medicinal Chemistry, Andrejus Korolkovas ;,II Ed. ,Wiely India, 2008
2. Medicinal Chemistry: A molecular and Biochemical approach; Thomas Nogrady,Donald F.Weaver;III Ed.:Oxford University Press , 2007

M.Sc. CHEMISTRY(With specialization in Analytical Chemistry) - IV SEMESTER

SAC846: ENVIRONMENTAL AND INDUSTRIAL MATERIAL ANALYSIS

Hours per week: 4

Semester End Examination: 60 Marks

Credits: 4

Continuous Evaluation: 40 marks

UNIT-I

Analysis of oils, fats, soaps and detergents

Introduction to natural fats and oils, Analysis of oils and fats: Softening point, Titre point, cloud point, Polenske value, Elaiden test. Saponification number. Iodine number and acid number. Introduction to soaps, analysis of soap (saponifiable and unsaponifiable), estimation of free alkali in soap.

UNIT-II

Analysis of Dyes and Paints

Types of dyes and their analysis, Composition and analysis of paints - determination of volatile and non-volatile constituents, flash points, separation of pigments, estimation of binders and thinners, total lead, lead chromate.

UNIT III

Analysis of Fertilizers and detergents.

- (a) Analysis of fertilizers: Ammonical fertilizers, phosphate fertilizers: determination of moisture, total N, NH_3 P, Si, lime.
4. Classification of detergents: Analysis of active ingredients from detergents, estimation of CMC, chlorides and total phosphates

UNIT-IV

Assessment of Water Quality—Sources of water, sampling procedure of water and waste water, classification of water for different uses, types of water pollutants and water quality standards for drinking water. Analytical methods for the determination of the following ions in water: Anions: CO_3^{2-} , HCO_3^- , F^- , Cl^- , SO_4^{2-} , PO_4^{3-} , NO_3^- , NO_2^- , Cations: Fe^{2+} , Fe^{3+} , Ca^{2+} , Mg^{2+} , Cr^{3+} . Determination of Dissolved Oxygen (D.O), Biochemical Oxygen Demand (BOD) and Chemical Oxygen Demand (COD).

UNIT-V

Assessment of Air Quality & soil: Composition of pure air, classification of air pollutants, sources of air pollutants, sampling of air, standards for ambient air quality.

Chemical analysis for the following:

Carbon monoxide (CO), Sulphur dioxide (SO_2), Hydrogen Sulfide (H_2S), Nitric oxide (NO).

Particulate matter - Suspended particulate matter (SPM) and Ozone

Analysis of soils: Sampling, determination of moisture, total N, P, Si, CaCO_3 , organic carbon and alkali metal ions

Textbooks:

1. Air pollution – M.N.Rao, H.V.N.Rao, Tata McGrawHill publishing company, 1998
1. Environmental Chemistry, Anil Kumar De, Wiley Eastern Ltd, 2003.
2. Environmental Analysis, S.M. Khopkar (IIT, Bombay), 1991.
3. Technical Methods of Analysis-Griffin, McGraw Hill Book, 1927
4. Text book of Metallurgical Analysis, B.C.Agarwal and S.P.Jain, Khanna publishers, 2003

Reference Books:

1. Standard Methods of Chemical Analysis, 6th edition, N. Howell Furman, D. Van Nostard Company Inc, Princeton, 1962

M.Sc. CHEMISTRY (Specialization in Organic Chemistry) - IV SEMESTER
SOC846: ASYMMETRIC SYNTHESIS

Hours per week: 4

Credits: 4

Semester End Examination: 60 Marks

Continuous Evaluation: 40 marks

Preamble

This course is designed to introduce the students about fundamentals of asymmetric synthesis, Chiral starting materials and chiral auxiliaries, Asymmetric alkylation, Asymmetric oxidations and Asymmetric reductions

Course Objectives

- To explain the fundamentals of asymmetric synthesis
- To explain the chiral starting materials and chiral auxiliaries
- To explain the Asymmetric alkylation with some specific reactions
- To explain the Asymmetric oxidations
- To explain the Asymmetric reductions

UNIT-I

Fundamentals of asymmetric synthesis: Terms, definitions and concepts in asymmetric synthesis. Introduction to chirality, phenomenon of chirality, types of chiral compounds, stereogenic centre, centrally and axially chiral compounds of carbon, prochirality, enantiotropic and diastereotopic isomers. Chiral compounds with more than one chiral centre. Biological significance of chirality. Selective synthesis of diastereomers and enantiomers.

Learning Outcome

At the end of the unit, the student will be able to know:

- basics of asymmetric synthesis,
- stereogenic centre
- Chiral compounds with more than one chiral centre,
- Biological significance of chirality

UNIT-II Chiral starting materials and chiral auxiliaries: Amino acids, sugars and hydroxy acids as chiral auxiliary. Nucleophile bearing a chiral auxiliary, chiral enolate, asymmetric aldol reactions. Electrophiles bearing chiral auxiliaries, asymmetric Michael addition, asymmetric addition to carbonyl compounds.

Learning Outcome

At the end of the unit, the student will be able to know:

- Chiral starting materials and chiral auxiliaries
- Nucleophile bearing a chiral auxiliary
- Electrophiles bearing chiral auxiliaries

UNIT-III Asymmetric alkylation: Chiral auxiliaries in concerted reactions-Diels alder reaction, Claisen-Cope rearrangement, asymmetric 2+2 cycloaddition, asymmetric formation of alkene double bonds.

Learning Outcome

At the end of the unit, the student will be able to know:

- Chiral auxiliaries in concerted reactions
- Rearrangement
- asymmetric formation of alkene double bonds.

UNIT-IV

Asymmetric oxidations: Mechanism of the sharpless asymmetric epoxidation, Sharpless asymmetric dihydroxylation, Jacobsen- Katsuki epoxidation, asymmetric oxidation of thioethers, chiral oxiaziridines and their uses.

Learning Outcome

At the end of the unit, the student will be able to know the Mechanism of:

- Sharpless asymmetric epoxidation, and dihydroxylation,
- Jacobsen- Katsuki epoxidation
- chiral oxiaziridines

UNIT-V

Asymmetric reductions: Catalytic hydrogenation with chiral transition metal complexes, asymmetric hydroboration of alkenes asymmetric reductions using chiral boranes and borohydrides, chirally modified LiAlH_4 .

Learning Outcome

At the end of the unit, the student will be able to know:

- Catalytic hydrogenation with chiral transition metal complexes
- asymmetric reductions using chiral boranes

Textbooks:

1. Asymmetric synthesis-Principles and methodology, 2nd Ed. by Y Vatsala, New age International, 2014.
2. Fundamentals of Asymmetric synthesis by G L David Krupadanam; Universities Press India Ltd, 2013
3. Advanced Organic Chemistry by Jerry March , 3rd Ed., Weastern, 2006

Reference books:

1. Asymmetric synthesis edited by Alan Aitken and, S.N. Kilenvi Blakie academic and Professional, 1992
2. Catalytic asymmetric synthesis edited by Iwao Ojima John Wiley & Sons, 2012
3. Advanced Asymmetric Synthesis edited by G.R.Stephenson; Chapman & Hall, 1996

M.Sc. CHEMISTRY (With specialization in Analytical Chemistry)- IV SEMESTER
SAC822: QUANTITATIVE ANALYSIS LAB

Hours per week: 9

Credits: 3

Semester End Examination: 60 Marks

Continuous Evaluation: 40 marks

1. Redox titrations of determination of ascorbic acid
2. Determination of total alkalinity of soda ash.
3. Determination of chlorides by Mohr's method, Fajan's method and Volhard's method.
4. Determination of manganese in pyrolusite by oxalate method.
5. Analysis of total Iron in ore by reduction with stannous chloride.
6. Complexometric titration for the analysis of limestone and dolomite with EDTA.
7. Estimation of the purity of oxalic acid employing standard Ce (IV) solution.
8. Determination of purity of ammonium chloride.
9. Determination of iodine in iodized salt
10. Coal analysis for moisture, ash, volatile matter and fixed carbon.
11. Gravimetric determination of chloride.
12. Gravimetric determination of sulphate
13. Determination of Cr (VI) using Diphenyl carbazide
14. Determination of Fe (II) using 1,10-Phenanthroline
15. Determination of Dissolved Oxygen
16. Determination of Sodium and potassium in a mixture by flame photometry

M.Sc. CHEMISTRY (Specialization in Analytical Chemistry) - IV SEMESTER
SCY822: Chromatographic Separation and Spectroscopy Lab-2

Hours per week: 6

Credits: 2

Semester End Examination: 60 Marks

Continuous Evaluation: 40 marks

Chromatography:

Separation and purification of organic compounds by Column Chromatography.

Spectrophotometry:

1. Determination of nitrite Using NEDA in selected samples.
2. Determination of phosphate using ammonium molybdate in selected samples.
3. Determination of Aspirin
4. Determination of Sulphates
5. Determination of ascorbic acid
6. Determination of Caffeine in an Analgesic Tablet by Ultraviolet Spectrophotometry
7. Determination of tannin

Demonstration Experiments

Determination of Zinc, Lead, and Copper by atomic absorption spectroscopy
Assay of organic compound by High performance liquid chromatography

M.Sc. CHEMISTRY(Specialization in Organic Chemistry) - IV SEMESTER
SOC822: QUALITATIVE ANALYSIS LAB

Hours per week: 9
Credits: 3

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Chemical separation of organic binary mixtures and systematic qualitative analysis of the organic compounds and preparation of two derivatives for each compound.

M.Sc. CHEMISTRY (Specialization in Organic Chemistry) - IV SEMESTER
SCY822: Chromatographic Separation and Spectroscopy Lab-2

Hours per week: 6
Credits: 2

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Chromatography:

Separation and purification of organic compounds by Column Chromatography.

Spectrophotometry:

1. Determination of nitrite Using NEDA in selected samples.
2. Determination of phosphate using ammonium molybdate in selected samples.
3. Determination of Aspirin
4. Determination of Sulphates
5. Determination of ascorbic acid
6. Determination of Caffeine in an Analgesic Tablet by Ultraviolet Spectrophotometry
7. Determination of tannin

Demonstration Experiments

Determination of Zinc, Lead and Copper by atomic absorption spectroscopy
Assay of organic compound by High performance liquid chromatography

M.Sc. Chemistry - IV SEMESTER
SCY 892: PROJECT WORK (Credits: 8)

Students are required to carry out a project in the fourth semester of their study, under the supervision of a faculty member of the department. The results are to be submitted in the form of a dissertation. Project work shall be evaluated by two examiners at the semester end examination

OPEN ELECTIVES OFFERED BY DEPARTMENT
(For admitted batch 2015-2016)

- 2) Fundamentals of Nanoscience and Technology (Semester -III)
- 3) Fundamentals of Chemical Analysis (Semester -III)
- 4) Chemistry in Day to day Life (Semester -III)
- 5) Concepts of instrumental methods and spectral data analysis for life sciences (Semester -III)

SOE 841: FUNDAMENTALS OF NANOSCIENCE AND NANOTECHNOLOGY
(w. e.f. 2019S-2020)

Hours per week: 3
Credits: 3

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Course objectives:

- ❖ *To understand the basic aspects of Nanoscience and Nanotechnology*
- ❖ *To acquire a knowledge in synthesis, properties and applications of nanomaterials*
- ❖ *To obtain an introductory knowledge of characterisation of nanomaterials*
- ❖ *To learn the role of nanomaterials and devices for biomedical and technological applications*

UNIT-I

Introduction: Concept of Size and Shape, difference between bulk and Nanomaterials; Definition of Nanomaterial; Classification of nanomaterials - Quantum dots, Nano wires, Nano tubes, 2D and 3D films; Carbon nanomaterials (CNT to Graphene); Mechanical, optical, and magnetic properties of nanomaterials.

Learning Outcomes: By the end of this unit, the student will able to

- *understand the fundamentals of nanoscience and nanotechnology*
- *classify various types of nanomaterials and its applications*

UNIT-II

General methods of preparation

Bottom Up and Top down Approaches - Sol-Gel chemical synthesis, Ultrasonication, Mechanical Milling, Chemical Vapour deposition (CVD) technique; Biological synthesis.

Learning Outcomes: By the end of this unit, the student will able to

- *understand synthesis methodology*
- *compare various types of synthesis strategies to prepare nanomaterials*

UNIT-III

Characterization techniques: X-ray diffraction technique, Scanning Electron Microscopy (SEM) Transmission Electron spectroscopy (TEM) and Atomic Force microscopy (AFM).

Learning Outcomes: By the end of this unit, the student will able to

- *understand the characterization principles of nanomaterials*
- *identify various methods suits to characterize the nanomaterials*

UNIT-IV

Biomedical applications: Materials for use in diagnostic and therapeutic applications – Gold nanoparticles, Silver nanoparticles Quantum dots, Magnetic nanoparticles; Diagnostic applications of immune-targeted nanoparticles; Targeted drug delivery.

Learning Outcomes: *By the end of this unit, the student will be able to*

- *understand the role of nanomaterials for biomedical application*
- *identify various types of nanomaterials for drug delivery applications*

UNIT-V

Energy and Environmental applications: The energy challenges - nano solar cells, making hydrogen fuel cells, hydrogen production and storage, saving energy with Lithium-ion batteries and LEDs; Cleaning air and keeping water crystal-clear with nanotechnology

Learning Outcomes: *By the end of this unit, the student will be able to*

- *understand various uses of nanomaterials for Energy applications*
- *list out various types of nanomaterials for purification of air and water*

Books:

1. Nanotechnology, Richard Booker, Earl Boysen, Wiley Publications, 2005
2. Nano: The Essentials, T. Pradeep, McGraw-Hill Education, 2010.
3. Nanochemistry: A chemical Approach to Nanomaterials, by G. A. Ozin, A. C. Arsenault & L. Cademartiri, RSC Publishing, 2008.

SOE 843: FUNDAMENTALS OF CHEMICAL ANALYSIS

Hours per week: 3
Credits: 3

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

UNIT-I

Statistical Treatment of Analytical Data and Sampling: Limitations of analytical methods. Classification of errors-systematic errors-sources, Random errors-sources and distribution. Accuracy and precision, Methods of determination of accuracy. Reliability of results-confidence interval. Comparison of results-Student's t-test, comparing the two means and standard deviations-F-test, t-test. Sampling and sample handling-representative sample, sample storage, sample pretreatment and sample preparation.

UNIT-II

Gravimetric analysis: General principles, stoichiometry, calculation of results from gravimetric data. Properties of precipitates, nucleation and crystal growth, factors influencing completion of precipitation. Co-precipitation and post-precipitation, purification and washing of precipitates. Precipitation from homogeneous solution, a few common gravimetric determinations-chloride as silver chloride, sulphate as barium sulphate.

UNIT-III

Acid base titrations: Principles of titrimetric analysis, titration curves for strong acid-strong base, weak acid-strong base and weak base-strong acid titrations, poly protic acids, determining the equivalence point-theory of acid base indicators, colour change range of indicator, selection of proper indicator, and applications of acid base titrations.

Acid-base titrations in non-aqueous solvents: Role of solvent in Acid-base titrations, solvent systems, some selected solvents, determining the equivalence point, typical applications-determination of carboxylic acids, phenols and amines.

UNIT-IV

Precipitation titrations: Titration curves, feasibility of precipitation titrations, factors affecting analyte concentration, completeness of the reaction, titrants and standards, indicators for precipitation titrations involving silver nitrate the Volhard, the Mohr and the Fajan's methods, typical applications.

UNIT-V

Complexometric titrations: Complex formation reactions, stability of complexes, stepwise formation constants, chelating agents, EDTA-acidic properties, complexes with metal ions, factors affecting the shape of titration curves-completeness of reaction, indicators for EDTA titrations-theory of common indicators, titration methods employing EDTA-direct, back and displacement titrations, selectivity, masking and demasking agents, typical applications of EDTA titrations-hardness of water for Calcium and magnesium

TEXT BOOKS

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th ed., 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 prentice Hall, Inc. New Delhi.
5. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint. 2003 Pearson Education Pvt. Ltd., New Delhi.

SOE 845: CONCEPTS OF INSTRUMENTAL METHODS AND SPECTRAL DATA ANALYSIS FOR LIFE SCIENCES

Hours per week: 3
Credits: 3

Semester End Examination: 60 Marks
Continuous Evaluation: 40 marks

Unit I

Sample Preparation Methods: Solid Phase extraction, Supercritical fluid extraction, Accelerated solvent extraction, Microwave extraction and Sonication.

Unit II

Optical Instrumentation Methods: Principle, instrumentation and relevant applications: Atomic absorption spectroscopy and Induced couple plasma spectroscopy.

Surface Analytical Technique: Basic Principle, Instrumentation and general applications: X-ray fluorescence spectroscopy.

Unit III

Electroanalytical Techniques: Principle, instrumentation and relevant applications: Ion selective electrodes and bio-sensors.

UNIT IV

Basics of Infrared spectroscopy and spectral analysis: Units of frequency wave length and wave number, the IR spectrometer, characteristic frequencies of various functional groups and interpretation of spectra

Basics of Nuclear Magnetic Resonance spectroscopy and spectral analysis: (Proton and Carbon –¹³ NMR) the chemical shift values of various characteristic protons and carbons, the intensity of NMR signals, spin-spin coupling to ¹³C-IH; IH-IH first order coupling: some simple IH-IH splitting patterns: the magnitude of IH-IH coupling constants.

Unit V

Basics of Mass spectroscopy: Basic Principles and instrumentation of mass spectrometer: Ionisation techniques and mass analyzers.

Hyphenated Techniques for Biological Samples: Principle, Instrumentation and relevant applications: LC – MS and GC- MS

Text books:

2. Instrumental methods of analysis - H.H. Willard, Meritt Jr. and J.A. Dean, CBS Publishers and distributors, 6th edition, 1986.
3. Principles of instrumental analysis – Douglas A. Skoog, F. James Holler and R. Crouch, Cengage Learning, 6th edition, 2006
5. Organic Spectroscopy, P.S .Kalsi, New-age International publication., 2007
6. Organic Spectroscopy, Y.R.Sharma, S.Chand Publication, 2014