CURRICULUM

and

SYLLABI OF COURSES

for

One Year **Undergraduate Certificate in Chemistry**,
Two-Years **Undergraduate Diploma in Chemistry**,
Three-Years **B.Sc. / B.Sc. (Hons.) in Chemistry**,
for
Four-Years **B.Sc. (Hons.) with Research in Chemistry**

[Exit Options after completion of 01 Year, 02 Years, 03 Years and 04 Years]

Applicable August 2022 Onwards

DEPARTMENT OF CHEMISTRY
SCHOOL OF PHYSICAL SCIENCES
DOON UNIVERSITY

PROGRAM OBJECTIVES

[1] To impart the key knowledge of chemical sciences and develop skills of conducting laboratory work/experiments to prepare the students for choosing careers in academia and/or industry in chemistry and related areas with strong scientific depth and temperament.

[2] To prepare students for higher studies in chemistry and the area of their choice.

PROGRAM OUTCOMES

[PO.1] Students will have a firm foundation in the fundamentals and application of current chemical and basic science including those in Physical, Organic, Inorganic, Analytical and Biochemistry, and other relevant and emerging fields of chemistry

[PO.2] Students will be able to seek new knowledge, skills and manage relevant information from various sources.

[PO.3] Students will be trained to work effectively and safely in the laboratory environment independently as well as in teams.

[PO.4] Students will be able to design and carry out scientific experiments as well as accurately draw logical inferences from the results of such experiments.

[PO.5] Students will be able to clearly communicate the results of scientific work in oral, written and ICT formats to both science community and society.

[PO.6] Students will be able to explain why chemistry is an integral activity for addressing social, economic, and environmental problems.

[PO.7] Students will be able to learn and act with integrity and good ethics in their profession and their obligation to society.

[PO.8] Students will be able to demonstrate knowledge and skills in analyzing and identifying entrepreneur opportunities.

COURSE STRUCTURE

FIRST SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
DSC	CYC-101	Atomic Structure & Chemical Bonding	3	0	1	4
DSC	CYC-102	Organo-analytical Techniques	3	0	1	4
DSC	CYC-103	Molecules in Motion & Ionic Equilibrium	3	0	1	4
*GE or *DSE	CYG-101	Choose from the pool of courses				4
*SEC	CYS-101	Choose one from the pool of courses				2
*AEC or *VAC		Choose one from the pool of courses				2
*AEC or *VAC		Choose one from the pool of courses				2
		Total Credits=				22

**DSE (Discipline Specific Elective) courses: The students are at liberty to choose this course from the list of Discipline Specific Elective (DSE) Courses given in Table 2 at succeeding pages or MOOC. *GE: Generic Elective Course: The students are at liberty to choose this course from the list of Generic Elective Courses given in Table 4 at succeeding pages or MOOC. *SEC (Skill Enhancement Course): The students are at liberty to choose this course from the list of Skill Enhancement Courses given in Table 5 at succeeding pages or MOOC. **VAC (Value Addition Courses): The students are at liberty to choose this course from the list of value addition courses (VAC) given in Table No. 6 on succeeding pages. **AEC (Ability Enhancement Course): The students are at liberty to choose this course from the list of Ability Enhancement Courses given in Table 7 at succeeding pages or MOOC.*

SECOND SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
DSC	CYC-151	Instrumentation of Basic Spectroscopic Techniques	3	1	0	4
DSC	CYC-152	Organic Hydrocarbons and Halo-compounds	3	0	1	4
DSC	CYC-153	Chemical Thermodynamics and its Applications	3		1	4
*GE or *DSE		Choose one from the pool of courses	3	0	1	4
*SEC		Choose one from the pool of courses				2
*AEC or *VAC		Choose one from the pool of courses				2
**AEC or **VAC		Choose one from the pool of courses				2
		Total Credits=				22

**DSE (Discipline Specific Elective) courses: The students are at liberty to choose this course from the list of Discipline Specific Elective (DSE) Courses given in Table 2 at succeeding pages or MOOC. *GE: Generic Elective Course: The students are at liberty to choose this course from the list of Generic Elective Courses given in Table 4 at succeeding pages or MOOC. *SEC (Skill Enhancement Course): The students are at liberty to choose this course from the list of Skill Enhancement Courses given in Table 5 at succeeding pages or MOOC. **VAC (Value Addition Courses): The students are at liberty to choose this course from the list of value addition courses (VAC) given in Table No. 6 on succeeding pages. **AEC (Ability Enhancement Course): The students are at liberty to choose this course from the list of Ability Enhancement Courses given in Table 7 at succeeding pages or MOOC.*

Note: Students will have an exit option after completion of two semester (i.e., one year with 44 credits) with Under Graduate Certificate in Science/Chemistry.

THIRD SEMESTER

Course Type	*Course Code*	*Course Title*	*L*	*T*	*P*	*C*
DSC	CYC−201	Chemistry of *s*- and *p*-Block Elements	3	0	1	4
DSC	CYC−202	Organic Compounds with Oxygen in Functional Groups	3	0	1	4
DSC	CYC−203	Phase Equilibria and Chemical Kinetics	3	0	1	4
*GE or *DSE		Choose one from the pool of courses	3	0	1	4
*SEC		Choose one from the pool of courses				2
*AEC or *VAC		Choose one from the pool of courses				2
*AEC or *VAC		Choose one from the pool of courses				2
		Total Credits=				22

**DSE (Discipline Specific Elective) courses: The students are at liberty to choose this course from the list of Discipline Specific Elective (DSE) Courses given in Table 2 at succeeding pages or MOOC. *GE: Generic Elective Course: The students are at liberty to choose this course from the list of Generic Elective Courses given in Table 4 at succeeding pages or MOOC. *SEC (Skill Enhancement Course): The students are at liberty to choose this course from the list of Skill Enhancement Courses given in Table 5 at succeeding pages or MOOC. **VAC (Value Addition Courses): The students are at liberty to choose this course from the list of value addition courses (VAC) given in Table No. 6 on succeeding pages. **AEC (Ability Enhancement Course): The students are at liberty to choose this course from the list of Ability Enhancement Courses given in Table 7 at succeeding pages or MOOC.*

FOURTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
DSC	CYC−251	Coordination Chemistry	3	0	1	4
DSC	CYC−252	Heterocyclic Chemistry	3	0	1	4
DSC	CYC−253	Electrochemistry	3	0	1	4
*GE or *DSE		Choose one from the pool of courses	3	0	1	4
*SEC		Choose one from the pool of courses				2
*AEC or *VAC		Choose one from the pool of courses				2
*AEC or *VAC		Choose one from the pool of courses				2
		Total Credits =				22

**DSE (Discipline Specific Elective) courses: The students are at liberty to choose this course from the list of Discipline Specific Elective (DSE) Courses given in Table 2 at succeeding pages or MOOC. *GE: Generic Elective Course: The students are at liberty to choose this course from the list of Generic Elective Courses given in Table 4 at succeeding pages or MOOC. *SEC (Skill Enhancement Course): The students are at liberty to choose this course from the list of Skill Enhancement Courses given in Table 5 at succeeding pages or MOOC. **VAC (Value Addition Courses): The students are at liberty to choose this course from the list of value addition courses (VAC) given in Table No. 6 on succeeding pages. **AEC (Ability Enhancement Course): The students are at liberty to choose this course from the list of Ability Enhancement Courses given in Table 7 at succeeding pages or MOOC.*

Note: Students will have an exit option after completion of four semester (i.e., two years with 88 credits) with Under Graduate Diploma in Science/Chemistry.

FIFTH SEMESTER

Course Type	*Course Code*	*Course Title*	*L*	*T*	*P*	*C*
DSC	CYC−301	Quantitative Inorganic Analysis and Synthesis Lab	3	0	1	4
DSC	CYC−302	Biomolecules	3	0	1	4
DSC	CYC−303	Quantum Chemistry	3	1	0	4
*GE or *DSE		Choose one from the pool of courses	3	0	1	4
*GE or *DSE		Choose one from the pool of courses	3	0	1	4
*SEC		Internship / Apprenticeship /Project / Community Outreach				2
		Total Credits =				22

**DSE (Discipline Specific Elective) courses: The students are at liberty to choose this course from the list of Discipline Specific Elective (DSE) Courses given in Table 2 at succeeding pages or MOOC. *GE: Generic Elective Course: The students are at liberty to choose this course from the list of Generic Elective Courses given in Table 4 at succeeding pages or MOOC. *SEC (Skill Enhancement Course): The students are at liberty to choose this course from the list of Skill Enhancement Courses given in Table 5 at succeeding pages or MOOC.*

SIXTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
DSC	CYC−351	Organometallic Chemistry	3	0	1	4
DSC	CYC−352	Stereochemistry, Carbohydrates, Dyes and Polymers	3	0	1	4
DSC	CYC−353	Molecular Spectroscopy and Photochemistry	3	0	1	4
*GE or *DSE		Choose one from the pool of courses				4
*GE or *DSE		Choose one from the pool of courses				4
*SEC		Internship / Apprenticeship /Project / Community Outreach’				2
		Total Credits =				22

**DSE (Discipline Specific Elective) courses: The students are at liberty to choose this course from the list of Discipline Specific Elective (DSE) Courses given in Table 2 at succeeding pages or MOOC. *GE: Generic Elective Course: The students are at liberty to choose this course from the list of Generic Elective Courses given in Table 4 at succeeding pages or MOOC. *SEC (Skill Enhancement Course): The students are at liberty to choose this course from the list of Skill Enhancement Courses given in Table 5 at succeeding pages or MOOC.*

Note: Student will have an exit option after completion of six semester (i.e., two years with 132 credits) with the degree of B.Sc. (Honours) in Science/Chemistry if he/she earns 80 credits (from 18 DSCs and 2 DSEs) in Chemistry

SEVENTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
DSC	CYC-401	Statistical Thermodynamics and Thermochemistry	3	0	1	4
*GE or *DSE		Choose one from the pool of courses				4
*GE or *DSE		Choose one from the pool of courses				4
*GE or *DSE		Choose one from the pool of courses				4
*SEC		Dissertation				6
Total Credits =						22

**DSE (Discipline Specific Elective) courses: The students are at liberty to choose this course from the list of Discipline Specific Elective (DSE) Courses given in Table 3 at succeeding pages or MOOC. *GE: Generic Elective Course: The students are at liberty to choose this course from the list of Generic Elective Courses given in Table 4 at succeeding pages or MOOC. *SEC (Skill Enhancement Course): It will be mandatory for the student to carry out dissertation which may be treated as Skill Enhancement Courses.*

EIGHTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
DSC	CYC-451	Pericyclic Reactions and Organic Photochemistry	3	0	1	4
*GE or *DSE		Choose one from the pool of courses				4
*GE or *DSE		Choose one from the pool of courses				4
*GE or *DSE		Choose one from the pool of courses				4
*SEC		Dissertation				6
		Total Credits =				22

**DSE (Discipline Specific Elective) courses: The students are at liberty to choose this course from the list of Discipline Specific Elective (DSE) Courses given in Table 3 at succeeding pages or MOOC. *GE: Generic Elective Course: The students are at liberty to choose this course from the list of Generic Elective Courses given in Table 4 at succeeding pages or MOOC. *SEC (Skill Enhancement Course): It will be mandatory for the student to carry out dissertation which may be treated as Skill Enhancement Courses.*

Note: Student will have an exit option after completion of eight semester (i.e., four years with 176 credits) with the degree of B.Sc. (Honours with Research) in Science/Chemistry [Major (Discipline 1 and Minor Discipline 2]

GUIDELINES

[1] Minimum Credit Requirements:

An academic credit is a unit by which the course work is measured. It determines the number of hours of instructions required per week. One credit is equivalent to one hour of teaching (lecture or tutorial) or two hours of practical work/field work per week.

For Under Graduate Certificate in Science/Chemistry

Course Type	Number of Courses	Credits
DSC (Discipline Specific Core Courses)	06 Courses	06 × 4 = 24
GE (Generic Elective) Courses *or* DSC (Discipline Specific Core) Courses *or* Generic Elective (GE) and Discipline Specific Elective (DSC)	02 Courses	02× 4 = 08
SEC (Skill Enhancement Course)	02 Courses: 02 Credits each	02 × 2 = 04
AEC (Ability Enhancement Courses) *or* VAC (Value Addition Courses) *or* AEC (Ability Enhancement Courses) and VAC (Value Addition Courses)	04 Courses: 02 Credits each	04 × 2 = 08
	Total Credits	**=44**

For Under Graduate Diploma in Science/Chemistry

Course Type	Number of Courses	Credits
DSC (Discipline Specific Core Courses)	12 Courses	12 × 4 = 48
GE (Generic Elective) Courses *or* DSC (Discipline Specific Core) Courses *or* Generic Elective (GE) and Discipline Specific Elective (DSC)	04 Courses	04× 4 = 16
SEC (Skill Enhancement Course)	04 Courses: 02 Credits each	04 × 2 = 08
AEC (Ability Enhancement Courses) *or* VAC (Value Addition Courses) *or* AEC (Ability Enhancement Courses) and VAC (Value Addition Courses)	08 Courses: 02 Credits each	08 × 2 = 16
	Total Credits	**= 88**

Degree of B.Sc. (Honours) in Science/Chemistry

Student will have to complete six semester (i.e., three years) and earn 132 credits for the degree of B.Sc. (Honours) in Science/Chemistry. In addition, he/she will have to ensure that he/she would earn 80 credits from 18 DSCs and 08 Credits from 2 DSEs) in Chemistry.

Course Type	Number of Courses	Credits
DSC (Discipline Specific Core Courses)	18 Courses	18 × 4 = 72
GE (Generic Elective) Courses *or* DSC (Discipline Specific Core) Courses *or* Generic Elective (GE) and Discipline Specific Elective (DSC)	08 Courses	08 × 4 = 32
SEC (Skill Enhancement Course)	06 Courses: 02 Credits each	06 × 2 = 12
AEC (Ability Enhancement Courses) *or* VAC (Value Addition Courses) *or* AEC (Ability Enhancement Courses) and VAC (Value Addition Courses)	08 Courses: 02 Credits each	08 × 2 = 16
	Total Credits	**=132**

B.Sc. (Honours with Research) in Science/Chemistry:
[Major (Discipline 1) and Minor (Discipline 2)]

Note: Student will have to complete eight semester (i.e., four years) with 176 credits credits for the degree of B.Sc. (Honours with Research) in Science/Chemistry. For the award of this degree, every student will have to earn 132 credits in first 03 years + 44 credits in remaining two semesters. In addition, he/she will have to ensure that he/she would earn 88 credits from 20 DSCs in Chemistry.

Course Type	Number of Courses	Credits
DSC (Discipline Specific Core Courses)	20 Courses	20 × 4 = 80
GE (Generic Elective) Courses *or* DSC (Discipline Specific Core) Courses *or* Generic Elective (GE) and Discipline Specific Elective (DSC)	14 Courses	14 × 4 = 56
SEC (Skill Enhancement Course)	06 Courses: 02 Credits each	06 × 2 = 12
Dissertation	06 Credits in Semester 7th and 06 Credits in 8th Semester	06 × 2 = 12
AEC (Ability Enhancement Courses) *or* VAC (Value Addition Courses) *or* AEC (Ability Enhancement Courses) and VAC (Value Addition Courses)	08 Courses: 02 Credits each	08 × 2 = 16
	Total Credits	**=176**

[2] Discipline Specific Core (DSC) Courses:

Every discipline shall offer three categories of courses of study, viz. Discipline Specific Core (DSC) courses, Discipline Specific Electives (DSE) courses and Generic Electives (GE).

Discipline Specific Core (DSC) courses represent those courses of Chemistry (Table 1), which should be pursued by a student as a mandatory requirement of his/her programme. These courses will be appropriately graded and arranged across the semesters of study, being undertaken by the student, with multiple exit options as per NEP 2020. Department or its relevant academic body will identify such courses and specify them in the framework of curriculum.

Table 1. List of Discipline Specific Core (DSC) Courses for the Students of Semester 1-8

S.No.	*Course Code*	*Course Title*	*Credits*
[1]	CYC-101	Atomic Structure & Chemical Bonding	04
[2]	CYC-102	Organo-analytical Techniques	04
[3]	CYC-103	Molecules in Motion and Ionic Equilibrium	04
[4]	CYC-151	Instrumentation of Basic Spectroscopic Techniques	04
[5]	CYC-152	Hydrocarbons, Haloalkanes and Haloarenes	04
[6]	CYC-153	Chemical Thermodynamics and Its Applications	04
[7]	CYC-201	S- and P-Block Elements	04
[8]	CYC-202	Organic Compounds with Oxygen in Functional Groups	04
[9]	CYC-203	Phase Equilibria and Chemical Kinetics	04
[10]	CYC-251	Coordination Chemistry	04
[11]	CYC-252	Heterocyclic Chemistry	04
[12]	CYC-253	Electrochemistry	04
[13]	CYC-301	Quantitative Inorganic Analysis and Synthesis Lab	04
[14]	CYC-302	Biomolecules	04
[15	CYC-303	Quantum Chemistry	04
[16]	CYC-351	Organometallic Chemistry	04
[17]	CYC-352	Stereochemistry, Carbohydrates, Dyes and Polymers	04
[18]	CYC-353	Molecular Spectroscopy and Photochemistry	04
[19]	CYC-401	Statistical Thermodynamics and Thermochemistry	04
[20]	CYC-451	Pericyclic Reactions and Organic Photochemistry	04

However, to pursue Honours degree programme in a 'Field of Multidisciplinary Courses of Study' such as B.Sc. (Honours) Life Sciences, the DSCs shall comprise of core credit courses of more than one discipline. For example, for B.Sc. (Honours) Life Sciences programme, a student shall study credit courses of three disciplines i.e., Botany, Zoology and Chemistry. In such a case, DSC 1 may be of Discipline A1 (say, Botany), DSC 2 may be of Discipline B 1 (say, Zoology) and DSC 3 may be of Discipline C 1 (say, Chemistry). However, the fourth year of such honours degree programme shall be devoted to the study of only one discipline

and hence the DSC courses in the VII and VIII semesters shall be of Discipline A/B/C and not a combination of these three disciplines.

[3] Discipline Specific Elective (DSE) Courses:

The Discipline Specific Elective (DSEs) courses represent those courses of Chemistry for which the students have the liberty to choose in different semesters. Department or its relevant academic body will identify and list such elective courses for the choice of the students. Such courses will be available for the students in case of single discipline programme as well as multidisciplinary programme. While pursuing B.Sc. (Honours) Chemistry, it will be mandatory for the student to choose the DSE from the pool of DSE courses of Chemistry. However, if the student is pursuing B.Sc. (Honours) in Life Sciences, he/she may choose the DSEs from the pools of courses of DSEs of Botany, Zoology and Chemistry, the core subjects for this programme of study. For completing Honours degree programme in a 'Field of Multidisciplinary Courses of Study' such as B.Sc. (Honours) Life Sciences, it will be mandatory for the student in the VII and VIII semesters (i.e., the fourth year of study) to choose DSEs from any one of the Disciplines A/B/C and not a combination of these three disciplines.

The list of Discipline Specific Elective (DSE) courses, offered by the Department of Chemistry, for the students of Semester 1-6 is as follows in Table 2. These courses will be non-semester specific. They may be offered in any semester depending upon the choice of the students and/or the availability of the resources and faculty members within the department.

Table 2. List of Discipline Specific Elective (DSE) Courses for the Students of Semester 1-6

S.No.	*Course Code*	*Title of Theory Course*	*Credits*
[1]	CYE-101	Polymer Chemistry *(Credits: 04)*	04
[2]	CYE-102	Inorganic Materials for Industrial Applications	04
[3]	CYE-103	Novel Inorganic Solids	04
[4]	CYE-104	Research Methodology for Chemistry	04
[5]	CYE-105	Applications of Computers in Chemistry	04
[6]	CYE-106	Molecular Modelling and Drug Design	04
[7]	CYE-107	Industrial Chemicals and Environment	04

The list of Discipline Specific Elective (DSE) courses, offered by the Department of Chemistry, for the students of Semester 7 and 8 is as follows in Table 3. These courses will be non-semester specific. They may be offered in either semester 7 or semester 8 depending upon the choice of the students and/or the availability of the resources and faculty members within the department.

Table 3. List of Discipline Specific Elective (DSE) Courses for the Students of Semester 7 and 8

S.No.	*Course Code*	*Title of Theory Course*	*Credits*
[1]	CYE-401	Synthetic Organic Chemistry Lab	04
[2]	CYE-402	Structure and Reactivity of Organic Molecules	04
[3]	CYE-403	Solid State Chemistry	04

[4]	CYE-404	Structure and Properties of Metal Complexes	04
[5]	CYE-405	Methods of Chemical Analysis	04
[6]	CYE-406	Reagents and Reactions in Organic Chemistry	04
[7]	CYE-407	Radiation and Photochemistry	04
[8]	CYE-408	Structure and Properties of Metal Complexes	04
[9]	CYE-409	Advanced Methods of Chemical Analysis	04
[10]	CYE-410	Frontiers in Bioinorganic Chemistry	04
[11]	CYE-411	Inorganic Photochemistry	04
[12]	CYE-412	Supramolecular Chemistry	04
[13]	CYE-413	Advanced Quantum Chemistry	04
[14]	CYE-414	Chemistry of Natural Products	04
[15]	CYE-415	Organic Structure Determination	04
[16]	CYE-416	Modern Organic Synthesis Methods	04
[17]	CYE-417	Medicinal Chemistry	04
[18]	CYE-418	Solid State Chemistry and Applications	04
[19]	CYE-419	Advanced Surface and Colloidal Chemistry	04
[20]	CYE-420	Environmental Pollutants and Analysis	04
[21]	CYE-421	Macromolecules and Nanomaterials	04
[22]	CYE-422	Green Methods of Synthesis	04
[23]	CYE-423	Total Organic Synthesis	04

[4] Generic Elective (GE) Courses:

Generic Elective (GE) courses represent those courses, which provide multidisciplinary or interdisciplinary approach in the education. The students will have the liberty to choose such courses in various other disciplines of study (excluding the GEs offered in the parent discipline). The Department would identify or prepare the GE courses and specify them in the framework. In case a student opts for DSEs beyond his/her discipline specific course(s) of study, such DSEs shall be treated as GEs for that student.

Department of Chemistry will offer the following Generic Elective (GE) courses (Table 4) for the students of other disciplines:

Table 4. List of Generic Elective Courses

S.No.	*Course Code*	*Title of The Course*	*Credits*
[1]	CYG−101	Atomic Structure, Chemical Bonding and Volumetric Analysis	04
[2]	CYG−102	General Organic Chemistry and Hydrocarbons	04
[3]	CYG−103	Chemical Energetics and Ionic Equilibria	04
[4]	CYG-104	Halogen and Oxygen Containing Organic Compounds	04
[5]	CYG-105	s- and p-Block Elements and Metallurgy	04
[6]	CYG-106	States of Matter and Chemical Kinetics	04
[7]	CYG-107	Chemistry of d-Block Elements	04
[8]	CYG-108	Spectroscopy and Photochemistry	04
[9]	CYG-109	Molecules of Life	04

[10]	CYG-110	Energy in Biosystem and Biochemistry Lab	04
[11]	CYG-111	Organometallics and Inorganic Synthesis	04
[12]	CYG-112	Organic Spectroscopic and Spectrometric Techniques	04
[13]	CYG-113	Bioinorganic Chemistry and Polynuclear Hydrocarbons	04
[14]	CYG-114	Phase Equilibrium, Conductance and Electrochemistry	04
[15]	CYG-115	Carboxylic Acids, Amines and Derivatives	04
[16]	CYG-116	Chemistry of Fuels and Pesticides	04

[5] Skill Enhancement Courses (SEC)

These are elective and skill-based courses (Table 5) in the field of chemical sciences. The students have a liberty to choose such courses from the pool. Objective of such courses is to provide the students with hands-on training, competencies and proficiency and skills. Department may offer some of such courses for the students of all other disciplines too. Such courses may also include Internship/ Apprenticeship/Project/ Community outreach (IAPC). The list of chemistry-based Skill Enhancement Courses is as follows:

Table 5. Skill Enhancement Courses (SEC)			
S.No.	*Course Code*	*Title*	*Credits*
[1]	CYS-101:	Fuel Chemistry	02
[2]	CYS-102	Basic Organic Synthesis Lab	02
[3]	CYS-103	Pesticide Chemistry	02
[4]	CYS-104	Chemistry of Cosmetics and Perfumes	02
[5]	CYS-105	IT Skills for Chemists	02
[6]	CYS-106	Chemical Technology and Society	02
[7]	CYS-107	Business Skills for Chemists	02
[8]	CYS-108	Cheminformatics	02
[9]	CYS-109	Intellectual Property Rights (IPR)	02
[10]	CYS-110	Analytical Clinical Biochemistry	02
[11]	CYS-111	Green Methods in Chemistry	02
[12]	CYS-112	Pharmaceutical Chemistry	02
[13]	CYS-113	Internship / Apprenticeship/Project / Community outreach (IAPC)	02
[14]	CYS-114	Internship / Apprenticeship/Project/ Community outreach (IAPC)	02
[15]	CYS-351	Minor Dissertation	04
[16]	CYS-401	Dissertation-I	06
[17]	CYS-451	Dissertation-II	06

[6] Value Addition Courses (VAC) and Ability Enhancement Courses (AEC)

These courses are also elective in nature. Students may choose such courses within the Department if Department offers. Otherwise, the students are at liberty to choose such courses and study them at other departments.

A student who desires to make Academic Project/Entrepreneurship as Minor has to pick the appropriate combination of courses of GE, SEC, VAC, & Internship/ Apprenticeship/Project/

Community (IAPC) which shall be offered in the form of various modules as specified in the scheme of studies.

(i) VAC courses are common pool of courses (Table 5) offered by different disciplines and aimed towards personality building; embedding ethical, cultural and constitutional values; promote critical thinking, indian knowledge systems, scientific temperament, communication skills, creative writing, presentation skills, sports & physical education and teamwork. These courses are meant for all round development of students.

Table 6. List of Value-Added Courses

Course Code	Course Title	L	T	P	C
DUV101	Universal Human Values and Professional Ethics	1		1	2
DUV102	Yoga and Naturopathy	1		1	2
DUV103	Indian Contribution to Science and Technology	1		1	2
DUV104	Family Culture and National Values	1		1	2
DUV105	Science of Happiness	1		1	2
DUV106	Environmental Communication	1		1	2
DUV107	Stage Acting	1		1	2

(ii) AEC courses are the courses (Table 6) based upon the content that leads to knowledge enhancement through various areas of study. They are Language and Literature and Environmental Science and Sustainable Development which will be mandatory for all disciplines.

Table 7. List of Ability Enhancement Compulsory Courses

Course Code	Course Title	L	T	P	C
DUA100	Environmental Studies	2			2
DUA101	English Language	2			2
DUA102	Spanish Language -I	2			2
DUA103	Spanish Language -II	2			2
DUA104	German Language- I	2			2
DUA105	German Language II	2			2
DUA106	French Language I	2			2
DUA107	French Language II	2			2
DUA108	Japanese Language-I	1	1		2
DUA109	Japanese Language-II	1	1		2
DUA110	Chinese Language-I	1	1		2
DUA111	Chinese Language-II	1	1		2
DUA201	Punjabi Language	2			2
DUA202	Sanskrit Language I	2			2
DUA203	Sanskrit Language II	2			2

DUA204	Malayalam: Language I	2			2
DUA205	Malayalam: Language II	2			2
DUA206	Tamil Language	2			2
DUA207	Bengali Language	2			2
DUA208	Telugu language	2			2

[6] Dissertation

Traditional teaching, usually based on lectures and tutorials, fosters the idea of instruction-driven learning model where students are passive listeners. However, project-based learning as a different learning paradigm is standing behind constructivism learning theory, where learning from real-world situations is put on the first place.

Students have a liberty to choose Dissertation (04 Credits) as a Discipline Specific Elective (DSE) course at 6th Semester. For the students who want to pursue B.Sc. with Research, it will be compulsory to carry out dissertation at 7th and 8th semesters.

First Semester

CYC−101: Atomic Structure & Chemical Bonding

Type	**:**	Core Course
Total Credits	**:**	04 (Theory: 03 + Practical: 01)
Total Hours	**:**	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[1] To know and understand atomic structure of elements, and various related principles and rules, periodic properties of elements, different types of chemical bonds including ionic bond, covalent bond, metallic bond and weak chemical forces

[2] To learn how to carry out the preparations of the solutions of different molarity/normality of titrants, titrimetric analysis, acid-base titrations, and oxidation-reduction titrimetric experiments

Course Outcomes:

After completion of this course,

[CO.1] Students will be able to understand the atomic structure of elements, and various related principles and rules, periodic properties of elements, different types of chemical bonds including ionic bond, covalent bond, metallic bond and weak chemical forces, and redox reactions and applications of electrode potential

[CO.2] Students will be able to carry out or perform the preparation of the solutions of different molarity/normality of titrants, titrimetric analysis, acid-base titrations and oxidation-reduction titrimetric experiments

COURSE CONTENT

Unit I: Atomic Structure:

Shapes of *s*, *p*, *d* and *f* orbitals.

Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number.

Unit II: Periodicity of Elements:

s, *p*, *d*, *f* block elements, the long form of periodic table. Detailed discussion of the following properties of the elements, with reference to *s* & *p*-block. Applications of ionization enthalpy Electron gain enthalpy, trends of electron gain enthalpy; Electronegativity, Pauling's/ Mulliken's/ Allred Rachow's/ and Mulliken-Jaffé's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. Sanderson's electron density ratio.

Unit III: Chemical Bonding:

(i) ***Ionic bond****:* General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy.

(ii) ***Covalent bond****:* Lewis structure, Valence Bond theory (Heitler-London approach). Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules N_2, O_2, C_2, B_2, F_2, CO, NO, and their ions; HCl, BeF_2, CO_2, (idea of s-p mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (σ and π bond approach) and bond lengths.

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization. Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

(iii) Metallic Bond: Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.

(iv) ***Weak Chemical Forces:*** van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Hydrogen bonding (theories of hydrogen bonding, valence bond treatment) Effects of chemical force, melting and boiling points, solubility energetics of dissolution process.

Unit IV: Laboratory Experiments

Lectures on principles involved in (i) volumetric analysis, (ii) acid base titrations and (iii) oxidation reduction titrimetry. Experiments:

A: Titrimetric Analysis

[1] To calibrate and use of apparatus
[2] To prepare the solutions of different molarity/normality of titrants

B: **Acid-Base Titrations**

[3] To estimate the carbonate and hydroxide present together in mixture.
[4] To estimate carbonate and bicarbonate present together in a mixture.
[5] To estimate free alkali present in different soaps/detergents

C: Oxidation-Reduction Titrimetry

[6] To estimate Fe(II) and oxalic acid using standardized $KMnO_4$ solution.
[7] To estimate oxalic acid and sodium oxalate in a given mixture.
[8] To estimate Fe(II) with $K_2Cr_2O_7$ using internal (diphenylamine, anthranilic acid) and external indicator.

Suggested Reading

[1] J. D. Lee: *A new Concise Inorganic Chemistry*, E L. B. S.
[2] F. A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
[3] Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
[4] James E. Huheey, Ellen Keiter and Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
[5] *Vogel's Qualitative Inorganic Analysis*, A.I. Vogel, Prentice Hall, 7th Edition.
[6] *Vogel's Quantitative Chemical Analysis*, A.I. Vogel, Prentice Hall, 6th Edition.

First Semester

CYC-102: Organo-analytical Techniques

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To be able to understand the fundamentals of UV-Vis, IR and NMR spectroscopy, interpret the data of UV-Vis, IR and NMR spectroscopic techniques in qualitative analysis and structural elucidation of organic compounds

[CO.2] To be able to elucidate the structures of organic compounds using the spectra obtained from UV-Vis, IR and NMR spectroscopic and mass spectrometric techniques.

Course Outcomes:

After completion of this course,

[CO.1] Students will be able to understand the fundamentals of UV-Vis, IR and NMR spectroscopy, and interpret the data of UV-Vis, IR and NMR spectroscopic techniques in qualitative analysis and structural elucidation of organic compounds.

[CO.1] Students will have the skills to elucidate the structures of organic compounds using the spectra obtained from UV-Vis, IR and NMR spectroscopic and mass spectrometric techniques.

COURSE CONTENT

Unit I:

General principles Introduction to absorption and emission spectroscopy.

Unit II: UV Spectroscopy

Types of electronic transitions, λmax, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of λ_{max} for the following systems: α,β unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); distinction between *cis* and *trans* isomers.

Unit III: IR Spectroscopy

Fundamental and non-fundamental molecular vibrations; IR absorption positions of O, N and S containing functional groups; Effect of H-bonding, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis.

Unit IV: NMR Spectroscopy

Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin – Spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Hydrogen deficiency index (HDI) or Index of unsaturation, Interpetation of NMR spectra of simple compounds.

Unit V: Mass Spectrometry

Mass spectrometry and its usefulness, Basic components and Functions of Mass Spectrometer, Mass Spectrum: molecular ion(s), and formation of fragments, molecular ion peak, base peak, radical cation, fragment ions, m/z ratio. Resolution, Atomic weight, Average mass, Monoisotopic mass, Exact mass, Nominal mass, Relative atomic mass, Use of mass spectral data in determining average relative atomic mass as well as relative molecular mass, application of high resolution mass spectrometry (HRMS) in the determination of molecular formula, Nitrogen rule, The rule of thirteen, Fragmentation patterns of

straight chain alkanes, Stevenson's rule, branched chain alkanes, alkenes, cycloalkenes, alkynes, aromatic hydrocarbons, alkyl-substituted aromatic hydrocarbons, aldehydes, ketones, Mc-Lafferty rearrangement, esters, carboxylic acids, amides, alcohols, phenols, ethers, haloalkanes, haloarenes, amines, nitriles and organic nitro compounds. Examples of mass spectrum of rubidium, lead, Cl_2, chloromethane, dichloromethane, methane, n-hexane, 2,2-dimethylhexane, 2-methyl pentane, iso-octane, n-decane, cyclohexane, trans-p-menthane, cis-2-pentene, 1-hexene, 1-pentene, n-octane, octene, 1-methyl-1-cyclohexene, 1-pentyne, 2-pentyne, toluene, p-xylene, propylbenzene, isopropylbenzene, n-butylbenzene, pentanal, m-tolualdehyde, 2-pentanone, propiophenone, *p*-chloroacetophenone, 2,4-dimethoxyacetophenone, cyclohexanone, ethyl butyrate, methyloctanoate, methyl o-toluate, pentanoic acid, *n*-decanoic acid, para-toluic acid, butyramide, benzamide, methyl alcohol, n-pentanol, 2-pentanol, 2-methyl-2-pentanol, 3-methyl-1-penten-3-ol, 4-methyl-1-penten-3-ol, cyclopentanol, phenol, benzyl alcohol, butyl methyl ether, anisole, 1-chloropropane, iso-propyl chloride, iso-propyl bromide, p-chlorotoluene, 1-bromobutane, p-bromotoluene, 3,4-dibromotoluene, iodobenzene, bromomethyl benzene (benzyl bromide), bromoethane, pentyl amine, dipropylamine, tripropyl amine, propionitrile, valeronitrile (pentanenitrile), 1-nitropropane, para-nitrotoluene and other simple organic molecules.

Unit VI:

Applications of IR, UV and NMR spectroscopic and mass spectrometric data for identification of simple organic molecules.

Unit VII: Laboratory Experiments

[1] To assess the miscibility or immiscibility of (i) water and acetone, (ii) water and dichloromethane (iii) water and petroleum ether (iv) petroleum ether and dichloromethane (vi) petroleum ether and acetone, (vii) dichloromethane and acetone

[2] To predict and practically observe the solubility of biphenyl, decanoic acid and 1-heptanol in water / petroleum ether

[3] To understand and find out the solubility of the given organic compound (acidic or basic) in 1M HCl and 1M NaOH aqueous solution

[4] To check the calibration of the thermometer, and determine the melting point of (i) naphthalene or some other compound, (ii) benzoic acid.

[5] To determine the melting point of the mixture of naphthalene with benzoic acid, and understand the effect of impurities on the melting point.

[6] To record and interpret the UV-Vis spectrum of given organic compound

[7] To record and interpret the IR spectrum of given organic compound

Suggested Readings

[1] P.S. Kalsi, "*Spectroscopy of Organic Compounds*" 9th Edition (2022), New Age Publishers.

[2] Jiben Roy, "*A Self-Study Guide to the Principles of Organic Chemistry*" Universal Publishers.

[3] Silverstein, R. M., Webseter, F. X. and Kiemle, D., *"Spectrometric Identification of Organic Compounds"*, 7th Ed., John Wiley &Sons.

[4] Kemp, W. L., *"Organic Spectroscopy"*, Palgrave.

[5] Pavia, D. L., *"Spectroscopy"*,4th Ed., Cengage.

[6] Williams, D. and Fleming, l., *"Spectroscopic Methods in Organic Chemistry"*, 6th Ed., McGraw Hill Education (India) Private Limited.

[7] Lab Manual, Li, Roy and Fortenberry

First Semester

CYC-103: Molecules in Motion and Ionic Equilibrium

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To be able to understand the kinetic molecular model of a gas, Maxwell distribution and its use in evaluating molecular velocities, behaviour of real gases, van der Waals equation of state and critical state of gases, physical properties of liquids, vapour pressure, surface tension and cleansing action of soaps and surfactants, nature of the solid state, elementary ideas of symmetry, symmetry elements and symmetry operations, defects in crystal structure X-ray diffraction and its application in crystal structure analysis, types of electrolytes, pH, buffers and buffer action and their applications in biochemical processes, acid base volumetric titrations

[CO.2] To be able to carry out the measurement of viscosity and surface tension of solutions using experimental techniques, the preparation of different pH buffers, and determine different chemical properties of acids and bases.

Course Outcomes:

After completion of this course,

[CO.1] Students will know and understand the kinetic molecular model of a gas, Maxwell distribution and its use in evaluating molecular velocities, behaviour of real gases, van der Waals equation of state and critical state of gases, physical properties of liquids, vapour pressure, surface tension and cleansing action of soaps and surfactants, nature of the solid state, elementary ideas of symmetry, symmetry elements and symmetry operations, defects in crystal structure X-ray diffraction and its application in crystal structure analysis, types of electrolytes, pH, buffers and buffer action and their applications in biochemical processes, acid base volumetric titrations

[CO.2] Students will have the skills to measure viscosity and surface tension of solutions using experimental techniques, prepare the solutions of different pH buffers, and determine different chemical properties of acids and bases.

COURSE CONTENT

Unit I: Gaseous State:

Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of σ from η; variation of viscosity with temperature and pressure critical state, relation between critical constants and van der Waals constants, law of corresponding states.

Unit II: Liquid state:

Qualitative treatment of the structure of the liquid state; Radial distribution function; physical properties of liquids; vapour pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity.

Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases.Qualitative discussion of structure of water.

Unit III: Ionic equilibria:

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono-, di-and triprotic acids (exact treatment).

Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical chemistry and biochemical processes in the human body.

Unit V: Laboratory Experiments:

A. Surface tension measurements.

[1] To determine the surface tension by (i) drop number (ii) drop weight method.
[2] To study the variation of surface tension of detergent solutions with concentration.

B. Viscosity measurement using Ostwald's viscometer.

[3] To determine the viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.
[4] To study the variation of viscosity of sucrose solution with the concentration of solute.

C. pH metry

[5] Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
[6] To prepare the buffer solutions of different pH
[7] To determine the dissociation constant of a weak acid.

Suggested Reading

[1] Atkins, P. W. & Paula, J. de Atkin's *Physical Chemistry* Ed., Oxford University Press 13 (2006).
[2] Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
[3] Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
[4] Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: Noida, UP (2009).
[5] Khosla, B. D.; Garg, V. C. & Gulati, A. Senior *Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
[6] Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry* 8th Ed.; McGraw-Hill: New York (2003).
[7] Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry* 3rd Ed.; W.H. Freeman & Co.: New York (2003).

Second Semester

CYC−151: Instrumentation of Basic Spectroscopic Techniques

Type	:	Core Course
Total Credits	:	04 (Theory: 04 + Practical: 0)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

Course Objectives:
[CO.1] To be able to understand the basic concepts of qualitative and quantitative analysis,
[CO.2] To be able to understand the principles and instrumentation of (i) various separation techniques (such as liquid chromatography, gas chromatography and electrophoresis), (ii) molecular (UV-vs and infrared) spectroscopy, and atomic spectroscopy.

Course Outcomes:
After completion of this course,
[CO.1] Students will know and understand the basic concepts of qualitative and quantitative analysis.
[CO.2] Student(s) will have the skills to handle the instrumental techniques including (i) separation techniques (such as liquid chromatography, gas chromatography and electrophoresis), (ii) molecular (UV-vs and infrared) spectroscopy, and atomic spectroscopy, (iii) electroanalytical methods (such as voltammetry and potentiometry), and (iv) thermal methods e.g., TGA, DSC and DTA

COURSE CONTENT

Unit I: Separation Techniques.

Chromatography: Introduction, Gas chromatography, liquid chromatography, supercritical fluids, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical field), Detection: simple vs. specific (gas and liquid). Detection as a means of further analysis (use of tags and coupling to IR and MS).

Unit II: Molecular spectroscopy:

Infrared spectroscopy:
Interactions of light with molecules: Absorption and Scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution), Fourier Transform (FTIR) and its advantages. Samples preparation methods and results expected. Applications and sample analysis.

UV-Visible/ Near IR: Emission, Absorption, Fluorescence and Photoaccoustic. Excitation sources (lasers, time resolution), wavelength dispersion (gratings, prisms, interference filters, laser, resolution), Detection of signal (photocells, photomultipliers, diode. arrays), sensitivity and S/N ratio, Single and Double Beam instruments, Interpretation (quantification, mixtures, absorption vs. fluorescence and the use of time, photoacoustic, fluorescent tags).

Unit III: Atomic Spectroscopy:

Atomic absorption, atomic emission, and atomic fluorescence. Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wavelength separation and resolution (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).

Unit III: Mass Spectrometry:

Principle and instrumentation, Ionization technique (electron impact, chemical ionization, electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, Detection and interpretation (how this is linked to excitation), interpretation of mass spectrum, effect of isotopes on appearance of mass spectrum; applications in molecular weight determination.

Suggested Readings

[1] *Principles of Instrumental Analysis* - 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
[2] *Instrumental Methods of Analysis*, 7th ed, Willard, Merritt, Dean, Settle.
[3] P.W. Atkins: *Physical Chemistry*.
[4] G.W. Castellan: *Physical Chemistry*.
[5] C.N. Banwell: *Fundamentals of Molecular Spectroscopy*.
[6] Brian Smith: *Infrared Spectral Interpretations: A Systematic Approach*.
[7] W.J. Moore: *Physical Chemistry*

Second Semester

CYC−152: Hydrocarbons, Haloalkanes and Haloarenes

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To be able to understand the nomenclature, shape, and geometry of organic molecules, various electronic effects that influence acidic or basic properties of molecules, electronic properties of various organic intermediates, their generation and reactivity, basic concepts of nucleophilic substitution, elimination and addition reactions.

[CO.2] To be able to understand the formation of carbon-carbon single bonds, double bonds and triple bonds, conformations of alkanes and cycloalkanes.

[CO.3] To be able to (i) purify the organic compounds using crystallization technique(s) (ii) to determine the melting points and boiling points of unknown organic compounds, and (iii) to separate the mixture of organic compounds using chromatography

Course Outcomes:

After completion of this course,

[CO.1] Students will be able to understand the nomenclature, shape, and geometry of organic molecules, various electronic effects that influence acidic or basic properties of molecules, electronic properties of various organic intermediates, their generation and reactivity, basic concepts of nucleophilic substitution, elimination and addition reactions.

[CO.2] Students will be able to understand the formation of carbon-carbon single bonds, double bonds and triple bonds, conformations of alkanes and cycloalkanes.

[CO.3] Students will be able to (i) purify the organic compounds using crystallization technique(s) (ii) to determine the melting points and boiling points of unknown organic compounds, and (iii) to separate the mixture of organic compounds using chromatography

COURSE CONTENT

Unit I: Basics of Organic Chemistry

Organic Compounds: Classification, and Nomenclature, Hybridization, Shapes of molecules, Influence of hybridization on bond properties.

Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and their applications; Dipole moment; Organic acids and bases; their relative strength.

Homolytic and Heterolytic fission with suitable examples. Curly arrow rules, formal charges; Electrophiles and Nucleophiles; Nucleophilicity and basicity; Types, shape and their relative stability of Carbocations, Carbanions, Free radicals and Carbenes.

Introduction to types of organic reactions and their mechanism: Addition, Elimination and Substitution reactions.

Unit II: Chemistry of Aliphatic Hydrocarbons:

A. Carbon-Carbon sigma bonds

Chemistry of alkanes: Formation of alkanes, Wurtz Reaction, Wurtz-Fittig Reactions, Free radical substitutions: Halogenation -relative reactivity and selectivity.

B. Carbon-Carbon pi bonds:

Formation of alkenes and alkynes by elimination reactions, Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations.

Reactions of alkenes: Electrophilic additions their mechanisms (Markownikoff/ Anti Markownikoff addition), mechanism of oxymercuration-demercuration, hydroborationoxidation, ozonolysis, reduction (catalytic and chemical), syn and anti-hydroxylation (oxidation). 1,2-and 1,4-addition reactions in conjugated dienes and, Diels-Alder reaction; Allylic and benzylic bromination and mechanism, e.g., propene, 1-butene, toluene, ethyl benzene.

Reactions of alkynes: Acidity, Electrophilic and Nucleophilic additions. Hydration to form carbonyl compounds, Alkylation of terminal alkynes.

C. Cycloalkanes and Conformational Analysis

Types of cycloalkanes and their relative stability, Baeyer strain theory, Conformation analysis of alkanes: Relative stability: Energy diagrams of cyclohexane: Chair, Boat and Twist boat forms; Relative stability with energy diagrams.

Unit III: Aromatic Hydrocarbons

Aromaticity: Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples. Electrophilic aromatic substitution: halogenation, nitration, sulphonation and Friedel-Craft's alkylation/acylation with their mechanism. Directing effects of the groups.

Unit IV: Chemistry of Halogenated Hydrocarbons:

Alkyl Halides*:* Methods of preparation, nucleophilic substitution reactions – S_N1, S_N2 and S_Ni mechanisms with stereochemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination.

Aryl Halides*:* Preparation, including preparation from diazonium salts. nucleophilic aromatic substitution; S_NAr, Benzyne mechanism.

Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Organometallic compounds of Mg and Li: Use in synthesis of organic compounds.

Unit V: Laboratory Experiments

[1] To determine the melting points of above compounds and unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)

[2] To purify benzoic acid by its crystallization in water

[3] To the boiling point of such liquid compounds which have boiling point lower than 100 °C (e.g., acetone) and more than 100 °C (e.g., toluene) by distillation and capillary method

[4] To separate acetone-toluene mixture using fractional distillation technique

[5] To study the rate of nucleophilic substitution reactions of primary alkyl halide (e.g., 1-bromobutane or some other compound), secondary alkyl halide (e.g., 2-bromobutane or some other organic compound) and tertiary alkyl halide (e.g., 2-bromo-2-methylpropane or some other organic compound) with sodium iodide (NaI) solution

[6] To study the rate of nucleophilic substitution reactions of primary alkyl halide (e.g., 1-bromobutane or some other compound), secondary alkyl halide (e.g., 2-bromobutane or some other organic compound) and tertiary alkyl halide (e.g., 2-bromo-2-methylpropane or some other organic compound) with alcoholic silver nitrate ($AgNO_3$ in EtOH) solution

[7] To generate nucleophiles of thiophenols or its derivatives and use such nucleophiles in carrying out nucleophilic substitution reactions

Suggested Readings

[1] P.S. Kalsi, "*Spectroscopy of Organic Compounds*" 9th Edition (2022), New Age Publishers.

[2] Jiben Roy, "*A Self-Study Guide to the Principles of Organic Chemistry*" Universal Publishers.

[3] P.S. Kalsi, "*Pharmaceutical Organic Chemistry*" (2022 Edition).

[4] Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)

[5] Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, Pearson.

Second Semester

CYC-153: Chemical Thermodynamics and Its Applications

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To be able to understand the laws of thermodynamics, chemical potential of an ideal mixture, thermodynamic equilibrium and spontaneous reactions, colligative properties of solutions and their applications in determination of molar masses

[CO.2] To be able to carry out the experimental determination of various thermodynamic and kinetic parameters of different chemical reactions

Course Outcomes:

After completion of this course,

[CO.1] Students will be able to understand the laws of thermodynamics, chemical potential of an ideal mixture, thermodynamic equilibrium and spontaneous reactions, colligative properties of solutions and their applications in determination of molar masses

[CO.2] Students will be to carry out the experimental determination of various thermodynamic and kinetic parameters of different chemical reactions

COURSE CONTENT

Unit I: Chemical Thermodynamics

Free Energy Functions: Gibbs and Helmholtz energy; variation of S, G, A with T, V, P; Free energy change and spontaneity. Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

Unit II: Systems of Variable Composition

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs-Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases.

Unit III: Chemical Equilibrium

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Coupling of exoergic and endoergic reactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration. Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants *Kp*, *Kc* and *Kx*. Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

Unit IV: Solutions and Colligative Properties

Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Excess thermodynamic functions.

Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure] and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

Unit V: Laboratory Experiments

(a) To determine heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).

(b) To determine heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.

(c) To calculate the enthalpy of ionization of ethanoic acid.

(d) To determine the heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.

(e) To determine the basicity/proticity of a polyprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.

(f) To determine the enthalpy of hydration of copper sulphate.

(g) To study the solubility of benzoic acid in water and determination of ΔH.

Suggested Readings

[1] Peter, A. & Paula, J. de. *Physical Chemistry* 9th Ed., Oxford University Press (2011).
[2] Castellan, G. W. *Physical Chemistry* 4th Ed., Narosa (2004).
[3] Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed., Prentice-Hall (2012).
[4] McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: Delhi (2004).
[5] Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. *Commonly Asked Questions in Thermodynamics*. CRC Press: NY (2011).
[6] Levine, I .N. *Physical Chemistry* 6th Ed., Tata Mc Graw Hill (2010).
[7] Metz, C.R. *2000 Solved Problems in Chemistry*, Schaum Series (2006)
[8] Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
[9] Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry* 8th Ed.; McGraw-Hill: New York (2003).
[10] Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry* 3rd Ed.; W.H. Freeman & Co.: New York (2003).

Third Semester

CYC-201: S- and P-Block Elements

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

Course Objectives:

[CO.1] To be able to understand general principles of metallurgy, different concepts and classification of acids and bases, chemistry of compounds of s- and p-block elements, noble gases and their compounds (such as fluorides of xenon)

[CO.2] To be able to understand the synthesis, structural aspects and applications of inorganic polymers including silicones, siloxanes, borazines, silicates and phosphazenes, and polysulphates.

Course Outcomes:

After completion of this course,

[CO.1] Student(s) will be able to understand general principles of metallurgy, different concepts and classification of acids and bases, chemistry of compounds of s- and p-block elements, noble gases and their compounds (such as fluorides of xenon).

[CO.2] Student(s) will be to understand the synthesis, structural aspects and applications of inorganic polymers including silicones, siloxanes, borazines, silicates and phosphazenes, and polysulphates.

COURSE CONTENT

Unit I: General Principles of Metallurgy

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy. Methods of purification of metals: Electrolytic Kroll process, Parting process, van Arkel-de Boer process and Mond's process, Zone refining.

Unit II: Acids and Bases

Brönsted-Lowry concept of acid-base reactions, solvated proton, relative strength of acids, types of acid-base reactions, levelling solvents, Lewis acid-base concept, Classification of Lewis acids, Hard and Soft Acids and Bases (HSAB) Application of HSAB principle.

Unit III: Chemistry of *s* and *p* Block Elements:

Inert pair effect, Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Complex formation tendency of *s* and *p* block elements.

Hydrides and their classification ionic, covalent and interstitial. Basic beryllium acetate and nitrate.

Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses.

Boric acid and borates, boron nitrides, borohydrides (diborane) carboranes and graphitic compounds, silanes, Oxides and oxoacids of nitrogen, Phosphorus and chlorine. Peroxo acids of sulphur, interhalogen compounds, polyhalide ions, pseudohalogens and basic properties of halogens.

Unit IV: Noble Gases:

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of XeF_2, XeF_4 and XeF_6; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF_2). Molecular shapes of noble gas compounds (VSEPR theory).

Unit V: Inorganic Polymers:

Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes. Borazines, silicates and phosphazenes, and polysulphates.

Suggested Readings

[1] Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
[2] Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. *Concepts & Models of Inorganic Chemistry* 3rd Ed., John Wiley Sons, N.Y. 1994.
[3] Greenwood, N.N. & Earnshaw. *Chemistry of the Elements*, Butterworth-Heinemann. 1997.
[4] Cotton, F.A. & Wilkinson, G. *Advanced Inorganic Chemistry*, Wiley, VCH, 1999.
[5] Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry* 4th Ed., Pearson, 2010.
[6] Shriver & Atkins, *Inorganic Chemistry* 5th Ed.

Third Semester

CYC-202: Organic Compounds with Oxygen in Functional Groups

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 15 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the basic concepts of stereochemistry, and methods of preparation and reactions of alcohols, phenols, ethers and epoxides.
[CO.2] To understand the structure, reactivity and preparation of carbonyl compounds.
[CO.3] To understand the methods of preparation and reactions of carboxylic compounds, acid chlorides, anhydrides, esters and amides.

Course Outcomes:

After completion of this course,
[CO.1] Student(s) will be able to understand basic concepts of stereochemistry, and methods of preparation and reactions of alcohols, phenols, ethers and epoxides.
[CO.2] Student(s) will understand the structure, reactivity and preparation of carbonyl compounds.
[CO.3] Student(s) will be able to understand the methods of preparation and reactions of carboxylic compounds, acid chlorides, anhydrides, esters and amides.

COURSE CONTENT

Unit I: Alcohols, Phenols, Ethers and Epoxides:

Alcohols*:* preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, Bouvaelt-Blanc Reduction; Preparation and properties of glycols: Oxidation by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement;
Phenols*:* Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer–Tiemann and Kolbe's–Schmidt Reactions, Fries and Claisen rearrangements with mechanism
Ethers and Epoxides*:* Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and $LiAlH_4$

Unit II: Carbonyl Compounds:

Structure, reactivity and preparation; Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisan-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, α-substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner, $LiAlH_4$, NaBH4, MPV, PDC and PGC);
Addition reactions of unsaturated carbonyl compounds: Michael addition.
Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

Unit III: Carboxylic Acids and their Derivatives:

Preparation, physical properties and reactions of monocarboxylic acids: Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids; Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic sustitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmannbromamide degradation and Curtius rearrangement.

Unit IV: Sulphur containing compounds:

Preparation and reactions of thiols, thioethers and sulphonic acids.

Unit V: Laboratory Experiments:

[1] To understand the principle and techniques of thin layer chromatography in separation and identification of curcumin, and curcumin in turmeric, based on comparisons with known reference standard and retention factors (R_f).

[2] To separate a mixture of two amino acids by ascending and horizontal paper chromatography

[3] To separate a mixture of two sugars by ascending paper chromatography

[4] To separate a mixture of o-and p-nitrophenol or o-and p-aminophenol by thin layer chromatography (TLC)

[5] To use chemical as well as spectroscopic methods to identify the presence (or absence) of (i) –COOH group in given organic compound (e.g., acetic acid), (ii) –OH group in given organic compound (e.g., 1-heptanol, phenol, salicylic acid, acetyl salicylic acid i.e., aspirin) (iii) >C=O group in given organic compound (e.g., cinnamaldehyde, pinacolone)

[6] To carry out aldol condensation of acetone and benzaldehyde

[7] To carry out the synthesis of pinacolone (a carbonyl compound) using pinacol (a diol) and sulphuric acid

Suggested Readings

[1] P.S. Kalsi, "*Spectroscopy of Organic Compounds*" 9th Edition (2022), New Age Publishers.
[2] Jiben Roy, "*A Self-Study Guide to the Principles of Organic Chemistry*" Universal Publishers.
[3] P.S. Kalsi, "*Pharmaceutical Organic Chemistry*" (2022 Edition).
[4] Lab Manual, Li, Roy and Fortenberry
[5] Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
[6] Finar, I. L. *Organic Chemistry* (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
[7] Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc.

Third Semester

CYC-203: Phase Equilibria and Chemical Kinetics

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To understand the concept of phases, phase diagram of one component system, the application of phase diagram, kinetics of reactions and experimental methods of determining rates of reactions.
[CO.2] To understand the types of catalysis, mechanisms of different catalysed reactions, types of adsorptions, adsorption isotherms and their applications, phase diagram of a three-component system and its application.
[CO.3] To understand the applications of distribution law.
[CO.4] To learn how to apply different method to monitor and understand kinetics of chemical reactions.

Course Outcomes:

After completion of this course,
[CO.1] Students will be able to understand the concept of phases, phase diagram of one component system, the application of phase diagram, kinetics of reactions and experimental methods of determining rates of reactions.
[CO.2] Student(s) will be able to understand the types of catalysis, mechanisms of different catalysed reactions, types of adsorptions, adsorption isotherms and their applications, phase diagram of a three-component system and its application.
[CO.3] Student(s) will be able to understand the applications of distribution law.
[CO.4] Student(s) will be able to apply different method to monitor and understand kinetics of chemical reactions.

COURSE CONTENT

Unit I: Phase Equilibria

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solidliquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems, with applications.

Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions.

Three component systems, water-chloroform-acetic acid system, triangular plots.

Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and nonideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation.

Nernst Distribution Law: its derivation and applications.

Unit II: Chemical Kinetics

Order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental methods of the determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions.

Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates.

Unit III: Catalysis

Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; effect of particle size and efficiency of nanoparticles as catalysts. Enzyme catalysis, Michaelis-Menten mechanism, acid-base catalysis.

Unit IV: Laboratory Experiments

[1] To determine critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.
[2] To understand the phase equilibria, and construct the phase diagram using cooling curves or ignition tube method: (a) simple eutectic and (b) congruently melting systems.
[3] To understand and determine the distribution of acetic/benzoic acid between water and cyclohexane.
[4] To study the equilibrium of at least one of the following reactions by the distribution method:

$I_2(aq) + I^- \rightarrow I_3^-(aq)^{2+}$

[5] To study the kinetics of the following reactions:

(1) Initial rate method: *Iodide-persulphate reaction*
(2) Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate.

Suggested Readings

[1] Peter Atkins & Julio De Paula, *Physical Chemistry* 9th Ed., Oxford University Press (2010).
[2] Castellan, G. W. *Physical Chemistry*, 4th Ed., Narosa (2004).
[3] McQuarrie, D. A. & Simon, J. D., *Molecular Thermodynamics*, Viva Books Pvt. Ltd.: New Delhi (2004).
[4] Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed., Prentice-Hall (2012).
[5] Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S.
[6] *Commonly Asked Questions in Thermodynamics*. CRC Press: NY (2011).
[7] Zundhal, S.S. *Chemistry concepts and applications* Cengage India (2011).
[8] Ball, D. W. *Physical Chemistry* Cengage India (2012).
[9] Mortimer, R. G. *Physical Chemistry* 3rd Ed., Elsevier: NOIDA, UP (2009).
[10] Levine, I. N. *Physical Chemistry* 6th Ed., Tata McGraw-Hill (2011).
[11] Metz, C. R. *Physical Chemistry* 2nd Ed., Tata McGraw-Hill (2009).
[12] Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
[13] Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
[14] Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York (2003).

Fourth Semester

CYC-251: Coordination Chemistry

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Tutorial: 01)
Total Hours	:	45 Theory + 15 Tutorial
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

Course Objectives:

[CO.1] To learn and know IUPAC nomenclature, isomerism, stereochemistry and various theories of coordination compounds.
[CO.2] To learn and know the general properties of transition elements, stability of different oxidation states of elements, chemistry of Ti, V, Cr Mn, Fe and Co in various oxidation states
[CO.3] To learn and know the properties of Lanthanoids and Actinoids
[CO.4] To learn and know the chemistry of metal ions present in biological systems

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will know and understand the IUPAC nomenclature, isomerism, stereochemistry and various theories of coordination compounds.
[CO.2] Student(s) will understand the general properties of transition elements, stability of different oxidation states of elements, chemistry of Ti, V, Cr Mn, Fe and Co in various oxidation states.
[CO.3] Student(s) will know and understand the properties of Lanthanoids and Actinoids,
[CO.4] Student(s) will know and understand the chemistry of metal ions present in biological systems

COURSE CONTENT

Unit I: Coordination Chemistry

Werner's theory, valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of 10 Dq (Δo), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (Δo, Δt). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory.

IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. Chelate effect, polynuclear complexes, Labile and inert complexes.

Unit II: Transition Elements

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer & Bsworth diagrams). Difference between the first, second and third transition series.

Chemistry of Ti, V, Cr Mn, Fe and Co in various oxidation states (excluding their metallurgy)

Unit III: Lanthanoids and Actinoids

Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only).

Unit IV: Bioinorganic Chemistry

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium / K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents in medicine.

Iron and its application in bio-systems, Haemoglobin; Storage and transfer of iron.

Suggested Readings

[1] Purcell, K.F & Kotz, J.C. *Inorganic Chemistry* W.B. Saunders Co, 1977.
[2] Huheey, J.E., *Inorganic Chemistry*, Prentice Hall, 1993.
[3] Lippard, S.J. & Berg, J.M. *Principles of Bioinorganic Chemistry* Panima Publishing Company 1994.
[4] Cotton, F.A. & Wilkinson, G, *Advanced Inorganic Chemistry*. Wiley-VCH, 1999
[5] Basolo, F, and Pearson, R.C., *Mechanisms of Inorganic Chemistry*, John Wiley & Sons, NY, 1967.
[6] Greenwood, N.N. & Earnshaw A., *Chemistry of the Elements*, Butterworth−Heinemann,1997.

Fourth Semester

CYC-252: Heterocyclic Chemistry

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To understand the organic compounds having nitrogen containing functional groups, and reactivity and basicity of alkyl and aryl amines.
[CO.2] To understand the structure and reactions of polynuclear hydrocarbons (such as naphthalene, phenanthrene and anthracene), and classification, nomenclature, and named synthesis of various heterocyclic compounds.
[CO.3] To understand natural occurrence, classification, synthesis and medicinal properties of alkaloids and terpenes.
[CO.4] To learn how to carry out the detection of extra elements and the presence or absence of nitro, amine and amide groups in the organic compounds.
[CO.5] To learn how to carry out qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols and carbonyl compounds).
[CO.6] To learn how to perform the chemical reaction(s) of amines with carbonyl compound derivatives of different polyaromatic hydrocarbons and heterocyclic compounds.

Course Outcomes:

After completion of this course,
[CO.1] Student(s) will be able to understand the organic compounds having nitrogen containing functional groups, and reactivity and basicity of alkyl and aryl amines.
[CO.2] Student(s) will be able to understand the structure and reactions of polynuclear hydrocarbons (such as naphthalene, phenanthrene and anthracene), and classification, nomenclature, and named synthesis of various heterocyclic compounds.
[CO.3] Student(s) will be able to natural occurrence, classification, synthesis and medicinal properties of alkaloids and terpenes.
[CO.4] Students will have the experimental skills to carry out the detection of extra elements and the presence or absence of nitro, amine and amide groups in the organic compounds.
[CO.5] Students will have the experimental skills to carry out qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols and carbonyl compounds).
[CO.6] Students will have the experimental skills to perform the chemical reaction(s) of amines with carbonyl compound derivatives of different polyaromatic hydrocarbons and heterocyclic compounds.

COURSE CONTENT

Unit I: Nitrogen Containing Functional Groups

Preparation and important reactions of nitro and compounds, nitriles and isonitriles.

Amines: Effect of substituent and solvent on basicity; Preparation and properties: Gabriel phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction; Distinction between 1°, 2° and 3° amines with Hinsberg reagent and nitrous acid.

Diazonium Salts: Preparation and their synthetic applications.

Unit II: Polynuclear Hydrocarbons

Reactions of naphthalene phenanthrene and anthracene Structure, Preparation and structure elucidation and important derivatives of naphthalene and anthracene; Polynuclear hydrocarbons.

Unit III: Heterocyclic Compounds

Classification and nomenclature, structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom; Synthesis, reactions and mechanism of substitution reactions of: Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Pyrimidine, Structure elucidation of indole, Fischer indole synthesis and Madelung synthesis), Structure elucidation of quinoline and isoquinoline, Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner-Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch
reaction
Derivatives of furan: Furfural and furoic acid.

Unit IV: Alkaloids

Natural occurrence, General structural features, Isolation and their physiological action Hoffmann's exhaustive methylation, Emde's modification, Structure elucidation and synthesis of Hygrine and Nicotine. Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine, and Reserpine.

Unit V: Terpenes

Occurrence, classification, isoprene rule; Elucidation of structure and synthesis of Citral, Neral and α-terpineol.

Unit VI: Laboratory Experiments

[1] To detect the presence (or absence) of extra elements in given organic compounds.
[2] To identify the presence (or absence) of groups such nitro, amine and amide groups by performing functional group tests in given organic compounds
[3] To carry out the nitration of methyl benzoate and obtain methyl *meta*-nitrobenzoate
[4] To carry out the reactions of amines with carbonyl compound derivatives of different polyaromatic hydrocarbons and heterocyclic compounds.
[5] To extract caffeine from tea leaves
[6] To carry out the reaction of 2,4-dinitrophenylhydrazine with given carbonyl compound

Suggested Readings

[1] Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
[2] Finar, I. L. *Organic Chemistry* (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
[3] Finar, I. L. *Organic Chemistry* (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
[4] Acheson, R.M. *Introduction to the Chemistry of Heterocyclic compounds*, John Welly & Sons (1976).
[5] Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc.
[6] Kalsi, P. S. *Textbook of Organic Chemistry* 1st Ed., New Age International (P) Ltd. Pub.
[7] Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry*, Oxford University Press.
[8] Singh, J.; Ali, S.M. & Singh, J. *Natural Product Chemistry*, Prajati Parakashan (2010).
[9] Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009).
[10] Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012)
[11] Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
[12] Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000).
[13] P.S. Kalsi, "*Spectroscopy of Organic Compounds*" 9th Edition (2022), New Age Publishers.
[14] Jiben Roy, "*A Self-Study Guide to the Principles of Organic Chemistry*" Universal Publishers.
[15] P.S. Kalsi, "*Pharmaceutical Organic Chemistry*" (2022 Edition).
[16] Lab Manual, Li, Roy and Fortenberry

Fourth Semester

CYC-253: Electrochemistry

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To understand the concepts of conductivity in electrolytes and dilute solutions, ionic velocities and ion mobility and methods of their determination

[CO.2] To understand different thermodynamic parameters for chemical reactions, comprehend the redox processes in electrochemical systems, applications of conductance measurement and laws of electrochemistry and their applications

[CO.3] To understand the chemical cells and applications of EMF measurements

[CO.4] To learn how to measure the conductance of the electrolytes using electroanalytical methods namely conductometry and potentiometry methods

[CO.5] To learn how to handle the electroanalytical techniques and explore their applications

Course Outcomes:

After completion of this course,

[CO.1] The students will have the ability to understand the concepts of conductivity in electrolytes and dilute solutions, ionic velocities and ion mobility and methods of their determination.

[CO.2] The students will have the ability to understand different thermodynamic parameters for chemical reactions, comprehend the redox processes in electrochemical systems, applications of conductance measurement and laws of electrochemistry and their applications.

[CO.3] The students will understand the chemical cells and applications of EMF measurements.

[CO.4] The students will have the experimental skills to measure the conductance of the electrolytes using electroanalytical methods namely conductometry and potentiometry methods.

[CO.5] The students will have the experimental skills to handle the electroanalytical techniques (i.e., conductometry and potentiometry) and explore their applications

COURSE CONTENT

Unit I: Conductance

Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules.

Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.

Unit II: Electrochemistry

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry.

Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different

kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and SbO/Sb_2O_3 electrodes. Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation).

Unit III: Laboratory Experiments

Conductometry

[1] To determine cell constant

[2] To determine equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

[3] To perform the following conductometric titrations:

[3.1] *Strong acid vs. strong base*

[3.2] *Weak acid vs. strong base*

[3.3] *Mixture of strong acid and weak acid vs. strong base*

[3.3] *Strong acid vs. weak base*

Potentiometry

[4] To perform and study the following potentiometric titrations:

[4.1] *Strong acid vs. strong base*

[4.2] *Weak acid vs. strong base*

[4.3] *Dibasic acid vs. strong base*

Suggested Readings

[1] Atkins, P.W & Paula, J.D. *Physical Chemistry*, 9th Ed., Oxford University Press (2011).

[12] Castellan, G. W. *Physical Chemistry* 4th Ed., Narosa (2004).

[13] Mortimer, R. G. *Physical Chemistry* 3rd Ed., Elsevier: NOIDA, UP (2009).

[14] Barrow, G. M., *Physical Chemistry* 5th Ed., Tata McGraw Hill: New Delhi (2006).

[5] Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed., Prentice-Hall (2012).

[6] Rogers, D. W. *Concise Physical Chemistry* Wiley (2010).

[7] Silbey, R. J.; Alberty, R. A. & Bawendi, M. G. *Physical Chemistry* 4th Ed., John Wiley & Sons, Inc. (2005)

[8] Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).

[9] Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).

[10] Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York (2003).

Fifth Semester

CYC-301: Quantitative Inorganic Analysis and Synthesis Lab

Type	:	Core Course
Total Credits	:	04 (Theory: 0 + Practical: 04)
Total Hours	:	120 Practical
Lectures	:	0 per week
Tutorial	:	0 per week
Practical	:	04 per week

Course Objectives:
[CO.1] To learn how to perform iodo / iodimetric titrations and gravimetric analysis
[CO.2] To learn how to carry out the preparations of inorganic and coordination compounds
[CO.3] To learn how to separate inorganic ions using chromatographic technique

Course Outcomes:
After completion of the course,
[CO.1] Student(s) will have the skills to perform iodo / iodimetric titrations and gravimetric analysis.
[CO.2] Student(s) will have the skills to carry out the preparations of inorganic and coordination compounds.
[CO.3] Student(s) will have the skills to separate inorganic ions using chromatographic technique.

COURSE CONTENT

Unit I: Iodo / Iodimetric Titrations

[1] To estimate Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodimetrically).
[2] To carry out the estimation of (i) *arsenite* and (ii) *antimony in tartar-emetic iodimetrically*
[3] To carry out the estimation of available chlorine in bleaching powder iodometrically.

Unit II: Gravimetric Analysis

[4] To carry out the quantitative estimation of nickel (II) using dimethylglyoxime (DMG).
[5] To carry out the quantitative estimation of copper as CuSCN.
[6] To carry out the quantitative estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$.
[7] To carry out the quantitative estimation of Al(III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminium oxinate).

Unit III: Inorganic Preparations

[8] To synthesize cuprous Chloride, [i.e., Cu_2Cl_2]
[9] To prepare manganese (III) phosphate, [i.e., $MnPO_4.H_2O$]
[10] To prepare aluminium potassium sulphate $KAl(SO_4)_2.12H_2O$ (Potash alum) or Chrome alum.
[11] To synthesize tetraamminecopper (II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$
[12] To synthesize *cis* and *trans* $K[Cr(C_2O_4)_2.(H_2O)_2]$ Potassium dioxalatodiaquachromate (III)
[13] To synthesize tetraamminecarbonatocobalt (III) ion
[14] To synthesize potassium tris(oxalate)ferrate(III)

Unit IV: Chromatography of Metal Ions

[15] To understand the principles (involved in chromatographic separations) and carry out the paper chromatographic separation of (a) Ni (II) and Co (II), and (b) Fe (III) and Al (III).

Suggested Readings

[1] Vogel, A.I. *A text book of Quantitative Analysis*, ELBS 1986.

Fifth Semester

CYC-302: Biomolecules

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the structures of genetic material DNA and RNA, the constituting nucleobases, nucleotides and their synthesis.
[CO.2] To know and understand the structure and classification of amino acids.
[CO.3] To know and understand the methods which are used for synthesizing the peptides and analysing the amino acids sequences.
[CO.4] To understand the classification, and mechanism of enzymes, and the factors influencing enzyme's activity, enzyme inhibitors and their importance.
[CO.5] To understand the classification and importance of fats, oil and lipids.
[CO.6] To understand the food metabolism, process of conversion of food into energy and use of energy in the synthesis of complex biomolecules.
[CO.7] To learn how to carry out the experiments for the estimation of glycine by Sorenson's formalin method, and also to study the titration curve of glycine.
[CO.8] To learn how to carry out the estimation of proteins using Lowry's method.
[CO.9] To learn how to study the action of salivary amylase on starch
[CO.10] To learn how to determine the saponification value of an oil or a fat.
[CO.11] To learn how to determine the iodine number of an oil/ fat.
[CO.12] To learn how to isolate and characterize the DNA from onion/ cauliflower/peas.

Course Outcomes:

After completion of the course,

[CO.1] The student(s) will be able to understand the structures of genetic material DNA and RNA, the constituting nucleobases, nucleotides and their synthesis.
[CO.2] The student(s) will be able to understand the amino acids.
[CO.3] Student(s) will know how to synthesize the peptides and analyse the amino acids sequences.
[CO.4] The student(s) will know about the classification, and mechanism of enzymes, and enzyme's activity, enzyme inhibitors and their importance.
[CO.5] The student(s) will understand the classification and importance of fats, oil and lipids.
[CO.6] The student(s) will know the food metabolism, process of conversion of food into energy and use of energy in the synthesis of complex biomolecules.
[CO.7] The student(s) will have the skills to carry out the experiments for the estimation of glycine by Sorenson's formalin method, and also to study the titration curve of glycine.
[CO.8] Student(s) will have the skills to carry out the estimation of proteins using Lowry's method.
[CO.9] The student(s) will have the skills to study the action of salivary amylase on starch
[CO.10] The student(s) will have the skills to determine the saponification value of an oil or a fat.
[CO.11] The student(s) will have the skills to determine the iodine number of an oil/ fat.
[CO.12] The student(s) will have the skills to isolate and characterize the DNA from onion/ cauliflower/peas.

COURSE CONTENT

Unit I: Nucleic Acids

Components of nucleic acids, Nucleosides and nucleotides;
Structure, synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine;
Structure of polynucleotides.

Unit II: Amino Acids, Peptides and Proteins

Amino acids, Peptides and their classification.

α-Amino Acids: Synthesis, ionic properties and reactions. Zwitterions, p*K*a values, isoelectric point and electrophoresis;

Study of peptides: determination of their primary structures-end group analysis, methods of peptide synthesis. Synthesis of peptides using N-protecting, C-protecting and C-activating groups -Solid-phase synthesis

Unit III: Enzymes

Introduction, classification and characteristics of enzymes. Salient features of active site of enzymes.

Mechanism of enzyme action (taking trypsin as example), factors affecting enzyme action, coenzymes and cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive and non-competitive inhibition including allosteric inhibition).

Unit IV: Lipids

Introduction to oils and fats; common fatty acids present in oils and fats, Hydrogenntion of fats and oils, Saponification value, acid value, iodine number. Reversion and rancidity.

Unit V: Concept of Energy in Biosystems

Cells obtain energy by the oxidation of foodstuff (organic molecules).

Introduction to metabolism (catabolism, anabolism).

ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change.

Agents for transfer of electrons in biological redox systems: NAD^+, FAD.

Conversion of Food to Energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle.

Overview of catabolic pathways of fat and protein.

Interrelationship in the metabolic pathways of protein, fat and carbohydrate.

Caloric value of food, standard caloric content of food types.

Unit VI: Laboratory Experiments

[1] To study the action of potato-cell enzyme (also known as polyphenol oxidase or PPO or catechol oxidase) on Catechol

[2] To study the action of potato-cell enzyme (also known as polyphenol oxidase or PPO or catechol oxidase) on hydrogen peroxide in acidic, alkaline and aqueous medium

[3] To carry out the estimation of glycine by Sorenson's formalin method.

[4] To study of the titration curve of glycine.

[5] To carry out the estimation of proteins by Lowry's method.

[6] To study the action of salivary amylase on starch at optimum conditions.

[7] To study the effect of temperature on the action of salivary amylase.

[8] To prepare soap and determine the saponification value of an oil or a fat.

[9] To determine the iodine number of an oil/ fat.

[10] To isolate and characterize DNA from onion/ cauliflower/peas.

[11] To perform qualitative tests on different biomolecules

Suggested Readings

[1] Berg, J.M., Tymoczko, J.L. and Stryer, L. (2006) *Biochemistry*. VIth Edition. W.H. Freeman and Co.

[2] Nelson, D.L., Cox, M.M. and Lehninger, A.L. (2009) *Principles of Biochemistry*. IV Edition. W.H. Freeman and Co.

[3] Murray, R.K., Granner, D.K., Mayes, P.A. and Rodwell, V.W. (2009) *Harper's Illustrated Biochemistry*. XXVIII edition. Lange Medical Books/ McGraw-Hill

[4] *Manual of Biochemistry* Workshop, 2012, Department of Chemistry, University of Delhi.

[5] Arthur, I. V. *Quantitative Organic Analysis*, Pearson.

[6] Lab Manual, Li, Roy & Fortenberry, University of Mississippi for Women.

Fifth Semester

CYC-303: Quantum Chemistry

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To understand and know the Schrodinger equation for a particle in a box and quantum chemical description.
[CO.2] To understand and know the Electronic and Hamiltonian operators for molecules.
[CO.3] To understand and know the quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
[CO.4] To understand the LCAO-MO treatment for H_2 molecule, Born-Oppenheimer approximation.
[CO.5] To understand and know the interaction of electromagnetic radiation with molecules and various types of spectra and their principles.
[CO.6] To understand and know the laws of photochemistry and concept of photochemical reactions and their role ion biochemical processes.

Course Outcomes:

After completing the course,
[CO.1] Students will know the Schrodinger equation for a particle in a box and quantum chemical description.
[CO.2] Student(s) will know the Electronic and Hamiltonian operators for molecules.
[CO.3] Student(s) will know the quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
[CO.4] Student(s) will know the LCAO-MO treatment for H_2 molecule, and Born-Oppenheimer approximation.
[CO.5] Student(s) will know the interaction of electromagnetic radiation with molecules and various types of spectra and their principles.
[CO.6] Student(s) will know the laws of photochemistry and concept of photochemical reactions and their role ion biochemical processes.

COURSE CONTENT

Unit I:

Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation and its application to free particle and "particle-in-a-box" (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wavefunctions, probability distribution functions, nodal properties, Extension to two- and three-dimensional boxes, separation of variables, degeneracy.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wavefunctions. Vibrational energy of diatomic molecules and zero-point energy.

Unit II: Angular momentum

Commutation rules, quantization of square of total angular momentum and z-component.

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution.

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus.

Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

Unit III: Chemical bonding

Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+. Bonding and antibonding orbitals. Qualitative extension to H_2. Comparison of LCAO-MO and VB treatments of H_2 (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic (BeH2, H2O) molecules. Qualitative MO theory and its application to AH2 type molecules.

Suggested Readings

[1] Chandra, A. K. *Introductory Quantum Chemistry* Tata McGraw-Hill (2001).
[2] House, J. E. *Fundamentals of Quantum Chemistry* 2nd Ed. Elsevier: USA (2004).
[3] Lowe, J. P. & Peterson, K. *Quantum Chemistry*, Academic Press (2005).
[4] McQuarrie, D.A, *Quantum Chemistry*, Viva Books Pvt. Ltd.

Sixth Semester

CYC-351: Organometallic Chemistry

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To understand and know the basics of organometallic compounds, their definition, their classification, 18 electron rule, EAN rule, hapticity of ligands, the properties of Zeise salt, metal alkyls and ferrocene, reaction kinetics and mechanism of substitution reactions in octahedral complexes and square planar complexes

[CO.2] To understand and know the applications of organometallic compounds as catalysts in different industrial processes

[CO.3] To learn how to use spectrophotometric method for the measurement of 10 Dq.

[CO.4] To learn how to verify the spectrochemical series.

[CO.5] To learn how to carry out controlled synthesis of two copper oxalate hydrate complexes on the basis of kinetic versus thermodynamic factors.

[CO.6] To learn how to prepare and synthesize acetylacetanato complexes of copper or iron and find out their λmax value experimentally.

[CO.7] To learn how to prepare and synthesize the ammine complexes of metal (such as nickel) and perform its ligand exchange reactions by substitution method.

Course Outcomes:

After completing the course,

[CO.1] Students will know and understand the basics of organometallic compounds, their definition, their classification, 18 electron rule, EAN rule, hapticity of ligands, the properties of Zeise salt, metal alkyls and ferrocene, reaction kinetics and mechanism of substitution reactions in octahedral complexes and square planar complexes

[CO.2] Students will know and understand the applications of organometallic compounds as catalysts in different industrial processes

[CO.3] Students will have the skills to use spectrophotometric method for the measurement of 10 Dq.

[CO.4] The students will have the skills to verify the spectrochemical series.

[CO.5] Students will have the skills to carry out controlled synthesis of two copper oxalate hydrate complexes on the basis of kinetic versus thermodynamic factors.

[CO.6] Students will have the skills to prepare and synthesize acetylacetanato complexes of copper or iron and find out their λmax value experimentally.

[CO.7] Students will have the skills to prepare and synthesize the ammine complexes of metal (such as nickel) and perform its ligand exchange reactions by substitution method.

COURSE CONTENT

Unit I: Organometallic Compounds

Definition and classification of organometallic compounds on the basis of bond type.

Concept of hapticity of organic ligands.

Metal Carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π-acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

Zeise's Salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler – Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium.

Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

Unit II: Reaction Kinetics and Mechanism

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans- effect, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, Thermodynamic and Kinetic stability, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedral complexes.

Unit III: Catalysis by Organometallic Compounds

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinsons Catalyst)
2. Hydroformylation (Co salts)
3. Wacker Process
4. Synthetic gasoline (Fischer Tropsch reaction)
5. Synthesis gas by metal carbonyl complexes

Unit VI: Laboratory Experiments

[1] To carry out measurement of 10 Dq by spectrophotometric method.
[2] To carry out the verification of spectrochemical series.
[3] To carry out the controlled synthesis of two copper oxalate hydrate complexes: kinetic vs thermodynamic factors.
[4] To prepare acetylacetanato complexes of $Cu^{2+/}Fe^{3+}$, and find the λ_{max} of the complex.
[5] To synthesize the ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

Suggested Readings

[1] Vogel, A.I. *Qualitative Inorganic Analysis*, Longman, 1972.
[2] Svehla, G. Vogel's *Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall, 1996-03-07.
[3] Cotton, F.A. G.; Wilkinson & Gaus, P.L. *Basic Inorganic Chemistry* 3rd Ed.; Wiley India.
[4] Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry*, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006.
[5] Sharpe, A.G. *Inorganic Chemistry*, 4th Indian Reprint (Pearson Education) 2005
[6] Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry* 3rd Ed., John Wiley and Sons, NY, 1994.
[7] Greenwood, N.N. & Earnshaw, A. *Chemistry of the Elements*, Elsevier 2nd Ed, 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
[8] Lee, J.D. *Concise Inorganic Chemistry* 5th Ed., John Wiley and sons 2008.
[9] Powell, P. *Principles of Organometallic Chemistry*, Chapman and Hall, 1988.
[10] Shriver, D.D. & P. Atkins, *Inorganic Chemistry* 2nd Ed., Oxford University Press, 1994.
[11] Basolo, F. & Person, R. *Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution* 2nd Ed., John Wiley & Sons Inc; NY.
[12] Crabtree, Robert H. *The Organometallic Chemistry of the Transition Metals*. j New York, NY: John Wiley, 2000.
[13] Spessard, Gary O., & Gary L. Miessler. *Organometallic Chemistry*. Upper Saddle River, NJ: Prentice-Hall, 1996.
[14] Vogel's *Qualitative Inorganic Analysis*, Revised by G. Svehla.
[15] Marr & Rockett *Inorganic Preparations*

Sixth Semester

CYC-352: Stereochemistry, Carbohydrates, Dyes and Polymers

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To learn and know monosaccharides, disaccharides, polysaccharides, dyes (synthesis and applications), polymers and polymerisation reactions

[CO.2] To learn how to carry out the extraction of caffeine from tea leaves.

[CO.3] To learn how to prepare (i) sodium polyacrylate, and (ii) urea formaldehyde, (iii) methyl orange.

[CO.4] To learn how to analyse carbohydrates (aldoses and ketoses), reducing and non-reducing sugars.

Course Outcomes:

After completing the course,

[CO.1] Students will learn and know monosaccharides, disacchharides, polysaccharides, dyes (synthesis and applications), polymers and polymerisation reactions

[CO.2] Students will have the skills to carry out the extraction of caffeine from tea leaves.

[CO.3] Students will have the skills to prepare (i) sodium polyacrylate, and (ii) urea formaldehyde, (iii) methyl orange.

[CO.4] Students will have the skills to analyse carbohydrates (aldoses and ketoses), reducing and non-reducing sugars.

COURSE CONTENT

Unit I: Stereochemistry:

Fischer Projection, Newmann and Sawhorse Projection formulae and their interconversions; Geometrical isomerism: cis–trans and, syn-anti isomerism E/Z notations with C.I.P rules. *Optical Isomerism:* Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers, Molecules with two or more chiral-centres, Distereoisomers, meso structures, Racemic mixture and resolution. Relative and absolute configuration: D/L and R/S designations.

Unit II: Carbohydrates

Occurrence, classification and their biological importance.

Monosaccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose, Haworth projections and conformational structures; Interconversions of aldoses and ketoses; Killiani-Fischer synthesis and Ruff degradation;

Disaccharides: Structure elucidation of maltose, lactose and sucrose.

Polysaccharides: Elementary treatment of starch, cellulose and glycogen.

Unit III: Dyes

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing.

Synthesis and Applications of:

Azo dyes: Methyl Orange and Congo Red (mechanism of Diazo Coupling);
Triphenyl Methane Dyes : Malachite Green, Rosaniline and Crystal Violet;
Phthalein Dyes : Phenolphthalein and Fluorescein;
Natural dyes : structure elucidation and synthesis of Alizarin and Indigotin;
Edible Dyes with examples.

Unit IV: Polymers

Introduction and classification including di-block, tri-block and amphiphilic polymers; Number average molecular weight, Weight average molecular weight, Degree of polymerization, Polydispersity Index.

Polymerisation reactions: Addition and condensation -Mechanism of cationic, anionic and free radical addition polymerization; Metallocene-based Ziegler-Natta polymerisation of alkenes; Preparation and applications of plastics – thermosetting (phenol-formaldehyde, Polyurethanes) and thermosoftening (PVC, polythene);

Fabrics: Natural and synthetic (acrylic, polyamido, polyester); Rubbers – natural and synthetic: Buna-S, Chloroprene and Neoprene; Vulcanization; Polymer additives; Introduction to liquid crystal polymers; Biodegradable and conducting polymers with examples.

Unit V: Laboratory Experiments

[1] To prepare (i) sodium polyacrylate, and (ii) urea formaldehyde.
[2] To analyse carbohydrates (aldoses and ketoses), reducing and non-reducing sugars.
[3] To carry out the preparation of methyl orange.
[4] To synthesize Aspirin (i.e., acetylsalicylic acid) by acetylation of salicylic acid.
[5] To carry out the extraction or isolation of active compounds (e.g., clove oil) from plant sources (such as cloves)
[6] To synthesize biodiesel
[7] To extract active pharmaceutical ingredient (API) from acetaminophen (paracetamol) tablet
[8] To synthesize acetaminophen (i.e., paracetamol) by acetylation of para-aminophenol

Suggested Readings

[1] Kalsi, P. S. *Textbook of Organic Chemistry* 1st Ed., New Age International (P) Ltd. Pub.
[2] Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
[3] Billmeyer, F. W. *Textbook of Polymer Science*, John Wiley & Sons, Inc.
[4] Gowariker, V. R.; Viswanathan, N. V. & Sreedhar, J. Polymer Science, New Age International (P) Ltd. Pub.
[5] Finar, I. L. *Organic Chemistry* (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
[6] Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc.
[7] Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry*, Oxford University Press.
[8] Singh, J.; Ali, S.M. & Singh, J. *Natural Product Chemistry*, Prajati Prakashan (2010).
[9] Kemp, W. Organic Spectroscopy, Palgrave
[10] Vogel, A.I. *Quantitative Organic Analysis*, Part 3, Pearson (2012).
[11] Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
[12] Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012)
[13] Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*: *Preparation and Quantitative Analysis*, University Press (2000).
[14] Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000).
[15] Lab manual of Li, Roy and Fortenberry, University of Mississipi for Women, USA
[16] P.S. Kalsi, "*Spectroscopy of Organic Compounds*" 9th Edition (2022), New Age Publishers.
[17] Jiben Roy, "*A Self-Study Guide to the Principles of Organic Chemistry*" Universal Publishers.
[18] P.S. Kalsi, "*Pharmaceutical Organic Chemistry*" (2022 Edition).

Sixth Semester

CYC-353: Molecular Spectroscopy and Photochemistry

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To be able to understand the interaction of electromagnetic radiation with molecules, principles of different molecular spectroscopies, laws of photochemistry and concept of photochemical reactions and their role ion biochemical processes.

[CO.2] To learn how to record and interpret UV-Vis Spectra of common chemicals.

[CO.3] To learn how to apply electronic spectroscopy in studying the kinetics of the reactions.

Course Outcomes:

After completing the course,

[CO.1] Student(s) will understand and know the interaction of electromagnetic radiation with molecules, principles of different molecular spectroscopies, laws of photochemistry and concept of photochemical reactions and their role ion biochemical processes.

[CO.2] Student(s) will have the skills to record and interpret UV-Vis Spectra of common chemicals.

[CO.3] Student(s) will have the skills to apply electronic spectroscopy in studying the kinetics of the reactions.

COURSE CONTENT

Unit I: Molecular Spectroscopy

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

Rotation Spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational Spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. *Vibration-rotation Spectroscopy*: diatomic vibrating rotator, P, Q, R branches.

Raman Spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Electronic Spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

Nuclear Magnetic Resonance (NMR) Spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low-resolution spectra, different scales, spin-spin coupling and high-resolution spectra, interpretation of PMR spectra of organic molecules.

Electron Spin Resonance (ESR) Spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

Unit II: Photochemistry

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws, of photochemistry, quantum yield, actinometry,

examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching. Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence. physiochemical processes, photostationary states, chemiluminescence.

Unit III: Laboratory Experiments on UV/Visible spectroscopy

[1] To study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values, and also to calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).
[2] To study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
[3] To record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water, and to discuss and comment on the effect of structure on the UV-spectra of organic compounds.

Unit IV: Laboratory Experiments on Colourimetry

[1] To verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration.
[2] To determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.
[3] To study the kinetics of iodination of propanone in acidic medium.
[4] To determine the dissociation constant of an indicator (phenolphthalein).
[5] To study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

Suggested Readings

[1] Banwell, C. N. & McCash, E. M. *Fundamentals of Molecular Spectroscopy* 4th Ed. Tata McGraw-Hill: New Delhi (2006).
[2] Chandra, A. K. *Introductory Quantum Chemistry* Tata McGraw-Hill (2001).
[3] House, J. E. *Fundamentals of Quantum Chemistry* 2nd Ed. Elsevier: USA (2004).
[4] Lowe, J. P. & Peterson, K. *Quantum Chemistry*, Academic Press (2005).
[5] Kakkar, R. *Atomic & Molecular Spectroscopy*, Cambridge University Press (2015).
[6] McHale, J. L *Molecular Spectroscopy*,2nd Ed. CRC Press (2017).
[7] Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
[8] Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry* 8th Ed.; McGraw-Hill: New York (2003).
[9] Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry* 3rd Ed.; W.H. Freeman & Co.: New York (2003).

7th Semester

CYC-401: Statistical Thermodynamics and Thermochemistry

(Core Course)

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Tutorial: 01)
Total Hours	:	45 Theory + 15 Tutorial
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

Course Objectives:

[CO.1] To know and understand statistical thermodynamics, theories and concepts related to activation energy and reaction rate, and thermodynamics of ionic systems

[CO.2] To know and understand types of reactions, and electron transfer dynamics

Course Outcomes:

After completing the course,

[CO.1] Students will know and understand statistical thermodynamics, theories and concepts related to activation energy and reaction rate, and thermodynamics of ionic systems

[CO.2] Students will know and understand the reactions, and electron transfer dynamics

COURSE CONTENT

Unit I: Statistical Thermodynamics

Concept of microstates and ensembles, microcanonical, canonical and grand canonical ensemble, average distribution, partition functions and its relation with thermodynamics properties, Maxwell Boltzmann, Bose-Einstein, Fermi-Dirac statistics, Molecular partition functions, translational, vibrational, and rotational partition functions. Ideal monoatomic and diatomic gases and their thermodynamic properties.

Unit II: Theories

Theoretical calculation of energy of activation using potential energy surface diagram, absolute reaction rate theory, comparison between gas phase and solution reactions

Unit III: Thermodynamics of Ionic Systems

Thermodynamics of reversible and irreversible electrochemical systems, thermodynamic foundation of theory of ionic interaction and calculation of energy of ionic interaction, interpretation of electrical conductance of electrolytes, thermodynamic treatment of diffusion potential.

Unit IV: Types of Reactions

Kinetics of chain reactions, detections of radical and kinetics of HBr, H_2O_2 reactions, explosion limits, elementary idea of unimolecular reactions, application of following to the reaction kinetics— solvent effect, kinetic isotope effect and salt effect, experimental technique for studying the fast reaction kinetics, kinetics of homogenous and heterogenous catalysis, kinetics of polymerization.

Unit V: Electron Transfer Dynamics

Electron transfer in homogeneous systems, theory of electron transfer processes, electron tunneling, experimental results, electron transfer in heterogeneous systems, study of kinetics of electrode processes.

Suggested Readings

[1] Seddon, J. M. and Gale, J. D., "*Thermodynamics and Statistical Mechanics*", Royal Society of Chemistry.
[2] McQuarrie, D. A. and Simon, J. D., "*Physical Chemistry*", Reprint, Viva Student Edition.
[3] McQuarrie, D. A. "*Statistical Mechanics*", Reprint, Viva Books Pvt. Ltd.
[4] Atkins, P. W., "*Physical Chemistry*", 7th Ed., ELBS, Oxford University Press.
[5] Silbey, R.J. and Alberty, R.A. "*Physical Chemistry*", 4th Ed., John Wiley & Sons, Inc., New York.
[6] West, R., "*Solid State Chemistry and its Applications*" Reprint, Wiley, India.
[7] Wells, A. F., "*Structural Inorganic Chemistry*", 5th edn., Clarendon Press, Oxford.
[8] Spaldin, N. "*Magnetic Materials: Fundamentals and Device Applications*", Cambridge University Press.

8th Semester

CYC-451: Pericyclic Reactions and Organic Photochemistry

Type	:	Core Course
Total Credits	:	04 (Theory: 03 + Tutorial: 01)
Total Hours	:	45 Theory + 15 Tutorial
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

Course Objectives:

[CO.1] To know and understand the classifications of pericyclic reactions, molecular orbital symmetry and frontier molecular orbital concepts.
[CO.2] To know and understand different electrocyclic reactions with even numbers of electron participation.
[CO.3] To know and understand sigmatropic rearrangements and their types in pericyclic reactions.
[CO.4] To know and understand photochemical reactions in organic chemistry.

Course Outcomes:

After completion of this course, the students will know and understand the classifications of pericyclic reactions, molecular orbital symmetry, frontier molecular orbital concepts, different electrocyclic reactions with even numbers of electron participation, Diels-Alder reaction, sigmatropic rearrangements and photochemical reactions in organic chemistry.

COURSE CONTENT

Unit I: Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. Conservation of orbital symmetry, State correlation diagrams, aromatic transition state (ATS) theory, generalized orbital symmetry (GOS) rule. Frontier Molecular Orbital (FMO) and Perturbation Molecular Orbital (PMO) approach.
Electrocyclic reaction; conrotatory and disrotatory motions, orbital correlation diagrams for 4n, 4n+2 and allyl systems, torquoselectivity.
Cycloaddition: antarafacial and suprafacialaddition, 4n and 4n+2 systems, 2+2 addition of ketenes , 1,3 dipolar cycloaddition, Diels-Alder Reaction and its variants, Cheleotropic and ene reactions.
Sigmatropic rearrangements: Suprafacial and Antarafacial shifts of H, [1,3], [1,5] shifts. Sigmatropic shifts involving carbon moieties, [3,3] shifts, Claisen rearrangement, aromatic Claisen rearrangement, Cope rearrangement, Oxy-cope rearrangement, Aza cope rearrangement, Carroll rearrangement, [5,5] shifts, [2,3] shifts. Curtius and Schmidt rearrangements.

Unit II: Organic Photochemistry

Quantum yields, intersystem crossing, photosensitization and energy transfer reactions. Photochemistry of olefins and carbonyl compounds, photo oxygenation and photo fragmentation, Photochemistry of aromatic compounds: isomerisation, additions and substitutions. Singlet molecular oxygen reactions. Patterno-Buchi reaction, Di-pimethane rearrangement, Bartons reaction and Photo-Fries rearrangement. Norrish I and II reactions.

Suggested Readings

[1] I. Fleming & John Wiley *"Frontier Orbital and Organic Chemical Reactions"* 1976.
[2] W. Carruthers *"Some modern Methods of Organic Synthesis"* Cambridge University Press, (1990).
[3] T.W. Greene, *"Protective Groups in Organic Synthesis"* Wiley-VCH, (1999)
[4] I. L. Finar, *"Organic Chemistry"*, Vol 11, ELBS (1968).
[5] Ward, *"Selectivity in Organic Synthesis"*, Wiley-VCH, 1999.
[6] S.Sankararaman, *"Pericyclic Reactions — A textbook"* Wiley-VCH, 2005.
[7] I. Fleming, *"Pericyclic Reactions"*, Oxford University Press (1999).
[8] I. Turro, V. Ramarnurthy & J. C. Scaiano, "*Modem molecular photochemistry of organic Compounds'*, University Science Books (2010).

Generic Elective Course: 04 Credits
(Non-Semester Specific)

CYG-101: Atomic Structure, Chemical Bonding and Volumetric Analysis

Type	:	Generic Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:
[CO.1] To understand the atomic structure, quantum mechanics, Schrodinger equation, various related principles and rules, periodic properties of elements, different types of chemical bonds, VSEPR theory, hybridization, molecular orbital theory, metallic bond and weak chemical forces.
[CO.4] To learn how to perform volumetric analysis using acid-base titrations and oxidation-reduction titrimetric experiments

Course Outcomes:
After completing the course,
[CO.1] Student(s) will be able to understand the atomic structure, quantum mechanics, Schrodinger equation, various related principles and rules, periodic properties of elements, different types of chemical bonds including ionic bond, covalent bond, VSEPR theory, hybridization, molecular orbital theory, metallic bond and weak chemical forces
[CO.2] Student(s) will have the experimental skills to perform volumetric analysis using acid-base titrations and oxidation-reduction titrimetric experiments

COURSE CONTENT

Unit I: Atomic Structure

Review of: *Bohr's theory and its limitations, dual behaviour of matter and radiation, de-Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to Atomic structure*.

What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of ψ and ψ^2, Schrödinger equation for hydrogen atom. Radial and angular parts of the hydogenic wavefunctions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation). Radial and angular nodes and their significance. Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals. Significance of quantum numbers, orbital angular momentum and quantum numbers m_l and m_s. Shapes of s, p and d atomic orbitals, nodal planes. Discovery of spin, spin quantum number (s) and magnetic spin quantum number (m_s).

Rules for filling electrons in various orbitals, electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations. (14 Lectures)

Unit II: Chemical Bonding and Molecular Structure

Ionic Bonding:

General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

Covalent bonding:

VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements.

Concept of resonance and resonating structures in various inorganic and organic compounds.

MO Approach:

Rules for the LCAO method, bonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1st and 2nd periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as CO, NO and NO^+. Comparison of VB and MO approaches. (16 Lectures)

Unit III: Volumetric Analysis and Laboratory Experiments

[1]. To perform estimation of Na_2CO_3 and $NaHCO_3$ present in a mixture.
[2]. To carry out estimation of oxalic acid by titrating it with $KMnO_4$.
[3]. To carry out the estimation of water of crystallization in Mohr's salt by titrating with KMnO4.
[4]. To carry out the estimation of Fe (II) ions by titrating it with $K_2Cr_2O_7$ using internal indicator.
[5]. To carry out the estimation of Cu (II) ions iodometrically using $Na_2S_2O_3$.

Suggested Readings

[1] J. D. Lee: *A new Concise Inorganic Chemistry*, E L. B. S.
[2] F. A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
[3] Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
[4] James E. Huheey, Ellen Keiter and Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
[5] Vogel's Qualitative Inorganic Analysis, A.I. Vogel, Prentice Hall, 7th Edition.
[6] Vogel's Quantitative Chemical Analysis, A.I. Vogel, Prentice Hall, 6th Edition.

Generic Elective Course: 04 Credits
(Non-Semester Specific)

CYG-102: General Organic Chemistry and Hydrocarbons

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:
[CO.1] To be able to understand the fundamentals of organic chemistry including (i) physical effects and electronic displacements, (ii) structure, shape and reactivity of organic molecules, (iii) stengths of organic acids and bases and methods of preparation and chemical properties of alkanes, alkenes and alkynes
[CO.2] To be able to understand the basic concepts of stereochemistry
[CO.3] To learn how to detect extra elements (N, S, Cl, Br, I) in organic compounds, (iii) to separate the mixtures of organic compounds using chromatography, and also to measure the R_f value.

Course Outcomes:
After completing the course,
[CO.1] Learners will be able to understand the fundamentals of organic chemistry including (i) physical effects and electronic displacements, (ii) structure, shape and reactivity of organic molecules, (iii) strengths of organic acids and bases and methods of preparation and chemical properties of alkanes, alkenes and alkynes
[CO.2] Learners will know and understand the basic concepts of stereochemistry
[CO.3] Learners will have the experimental skills to detect extra elements (N, S, Cl, Br, I) in organic compounds, and to separate the mixtures of organic compounds using chromatography, and also to measure the R_f value.

COURSE CONTENT

Unit I: Fundamentals of Organic Chemistry

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis. Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals. Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule.

Unit II: Stereochemistry

Conformations with respect to ethane, butane and cyclohexane. Interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations. Concept of chirality (upto two carbon atoms). Configuration: Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). Threo and erythro; D and L; cis - trans nomenclature; CIP Rules: R/ S (for upto 2 chiral carbon atoms) and E / Z Nomenclature (for upto two C=C systems). (10 Lectures)

Unit III: Aliphatic and Aromatic Hydrocarbons

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

Alkanes: (Upto 5 Carbons). Preparation: Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. Reactions: Free radical Substitution: Halogenation.

Alkenes: (Upto 5 Carbons) Preparation: Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); cis alkenes (Partial catalytic hydrogenation) and trans alkenes (Birch reduction). Reactions: cis-addition (alk. $KMnO_4$) and trans-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymecuration-demercuration, Hydroboration-oxidation.

Alkynes: (Upto 5 Carbons) Preparation: Acetylene from CaC_2 and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides. Reactions: formation of metal acetylides, addition of bromine and alkaline $KMnO_4$, ozonolysis and oxidation with hot alk. $KMnO_4$.

Preparation and Reactions of Aromatic Hydrocarbons (Case benzene): from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. Electrophilic substitution: nitration, halogenation and sulphonation. Friedel-Craft's reaction (alkylation and acylation) (upto 4 carbons on benzene). Side chain oxidation of alkyl benzenes (upto 4 carbons on benzene).

Unit IV: Laboratory Experiments

[1] To separate the mixtures by chromatography, and measure the R_f value in the given mixture of two compounds:

(1.1) Identify and separate the components of a given mixture of two amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by paper chromatography

(1.2) Identify and separate the sugars present in the given mixture by paper chromatography.

[2] To detect the presence or absence of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)

Suggested Readings

[1] Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
[2] T. W. Graham Solomon: *Organic Chemistry*, John Wiley and Sons.
[3] Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
[4] E. L. Eliel: *Stereochemistry of Carbon Compounds*, Tata McGraw Hill.
[5] I. L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
[6] R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
[7] Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand
[8] Vogel's *Quantitative Chemical Analysis*, A.I. Vogel, Prentice Hall, 6th Edition.
[9] Textbook of *Practical Organic Chemistry*, A.I. Vogel , Prentice Hall, 5th edition.
[10] F. G. Mann. & B. C. Saunders, *Practical Organic Chemistry*, Orient Longman, 1960.

Generic Elective Course: 04 Credits

CYG-103: Chemical Energetics and Ionic Equilibria

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To be able to understand thermodynamics and its laws, important principles and definitions of thermochemistry, important concepts of chemical equilibrium and ionic equilibrium.

[CO.2] To learn how to carry out the experimental determination of (i) the heat capacity of calorimeter (ii) enthalpies of different types of chemical reactions (such as neutralization, ionization and hydration), and (ii) the pH of different solutions using pH-meter.

Course Outcomes:

After completion of the course,

[CO.1] Learners will be able to understand and know the thermodynamics and its Laws, important principles and definitions of thermochemistry, important concepts of chemical equilibrium and ionic equilibrium.

[CO.2] Learners will have the experimental skills to carry out the experimental determination of (i) the heat capacity of calorimeter (ii) enthalpies of different types of chemical reactions (such as neutralization, ionization and hydration), and (ii) the pH of different solutions using pH-meter.

COURSE CONTENT

Unit I: Chemical Energetics

Review of thermodynamics and the Laws of Thermodynamics.

Important principles and definitions of thermochemistry. Concept of standard state and standard enthalpies of formations, integral and differential enthalpies of solution and dilution. Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data. Variation of enthalpy of a reaction with temperature – Kirchhoff's equation.

Statement of Third Law of thermodynamics and calculation of absolute entropies of substances.

Unit II: Chemical Equilibrium:

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between ΔG and ΔG^o, Le Chatelier's principle. Relationships between K_p, K_c and K_x for reactions involving ideal gases.

Unit III: Ionic Equilibria:

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

Unit IV: Laboratory Experiments

[1] To determine the heat capacity of calorimeter for different volumes.

[2] To determine the enthalpy of neutralization of HCl with NaOH.

[3] To determine the enthalpy of ionization of acetic acid.

[4] To determine the integral enthalpy of solution of salts (KNO_3, NH_4Cl).
[5] To determine the enthalpy of hydration of copper sulphate.
[6] To study the solubility of benzoic acid in water and determination of ΔH.
[7] To measure the pH of different solutions like aerated drinks, fruit juices, shampoos and soaps (use dilute solutions of soaps and shampoos to prevent damage to the glass electrode) using pH-meter.
[8] To prepare the buffer solutions: (i) Sodium acetate-acetic acid, and (ii) Ammonium chloride-ammonium hydroxide
[9] To measure the pH of buffer solutions and comparison of the values with theoretical values.

Suggested Readings

[1] G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).
[2] G. W. Castellan: *Physical Chemistry* 4th Edn. Narosa (2004).
[3] J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry* Cengage Lening India Pvt. Ltd., New Delhi (2009).
[4] B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).
[5] R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
[6] B.D. Khosla, *Senior Practical Physical Chemistry*, R. Chand & Co.

Generic Elective Course: 04 Credits

CYG-104: Halogen and Oxygen Containing Organic Compounds

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the methods of preparation and chemical properties of aromatic hydrocarbons, alkyl halides, aryl halides, alcohols, phenols, ethers, aldehydes and ketones

[CO.2] To know how to purify organic compounds by crystallization and to determine their melting and boiling points, and prepare some organic compounds using simple one or two-step reactions.

Course Outcomes:

After completion of the course,

[CO.1] Learners will be to understand and know the methods of preparation and chemical properties of aromatic hydrocarbons, alkyl halides, aryl halides, alcohols, phenols, ethers, aldehydes and ketones

[CO.2] Learners will have the experimental skills to (i) purify organic compounds by crystallization and determine their melting and boiling points, and (ii) prepare some organic compounds using simple one or two-step reactions.

COURSE CONTENT

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

Unit I: Alkyl and Aryl Halides

Alkyl Halides (Upto 5 Carbons)*:* Types of Nucleophilic Substitution (SN_1, SN_2 and SNi) reactions.

Preparation: from alkenes and alcohols.

Reactions: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation. Williamson's ether synthesis: Elimination vs substitution.

Aryl Halides: Preparation**:** (Chloro, bromo and iodo-benzene case): from phenol, Sandmeyer & Gattermann reactions.

Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by –OH group) and effect of nitro substituent. Benzyne Mechanism: KNH_2/NH_3 (or $NaNH_2/NH_3$).

Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

Unit II: Alcohols, Phenols and Ethers (Upto 5 Carbons)

Alcohols:

Preparation: Preparation of 1°, 2° and 3° alcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters.

Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. $KMnO_4$, acidic dichromate, conc. HNO_3). Oppeneauer oxidation

Diols: (Upto 6 Carbons) oxidation of diols. Pinacol-Pinacolone rearrangement.

Phenols: (Phenol case)

Preparation: Cumene hydroperoxide method, from diazonium salts. Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. Reimer-Tiemann Reaction, Gattermann-Koch Reaction, Houben–Hoesch Condensation, Schotten – Baumann Reaction.

Ethers (aliphatic and aromatic): Cleavage of ethers with HI.

Unit III: Aldehydes and Ketones (Aliphatic and Aromatic)

(Formaldehye, acetaldehyde, acetone and benzaldehyde).

Preparation: from acid chlorides and from nitriles.

Reactions – Reaction with HCN, ROH, $NaHSO_3$, NH_2-G derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Pondorff Verley reduction. (14 Lectures)

Unit IV: Laboratory Experiments

[1] To purify benzoic acid by crystallization in water
[2] To purify the mixture of acetone and toluene by distillation.
[2] To determine the melting and boiling points of organic compounds.
[3] To carry out the nitration reaction of methyl benzoate
[4] To prepare pinacolone from pinacol
[5] To carry out the aldol condensation reaction between acetone and benzaldehyde
[6] To carry out bromination of Phenol/Aniline.
[7] To carry out the benzoylation of amines/phenols
[8] To synthesize oxime and 2,4 dinitrophenylhydrazone of aldehyde/ketone

Suggested Readings

[1] T. W. Graham Solomons: *Organic Chemistry*, John Wiley and Sons.
[2] Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
[3] I.L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
[4] R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
[5] Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand.
[6] J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry* Cengage Lening India Pvt. Ltd., New Delhi (2009).
[7] B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).
[8] R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
[9] A.I. Vogel: *Textbook of Practical Organic Chemistry*, 5th edition, Prentice-Hall.
[10] F. G. Mann & B. C. Saunders, *Practical Organic Chemistry*, Orient Longman (1960).

Generic Elective Course: 04 Credits

CYG-105: s- and p-Block Elements and Metallurgy

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the chemistry of s and p block elements and their compounds including hydrides of nitrogen, oxoacids of P, S and Cl and halides and oxohalides

[CO.2] To know and understand the general principles of metallurgy, and methods of purification of metals

[CO.3] To learn how to perform semi-micro qualitative analysis for identifying cations and anions

Course Outcomes:

After completion of this course,

[CO.1] Student(s) will know and understand the chemistry of s and p-block elements and their compounds including hydrides of nitrogen, oxoacids of P, S and Cl and halides and oxohalides.

[CO.2] Student(s) will know and understand the general principles of metallurgy, and methods of purification of metals.

[CO.3] Student(s) will have the skills to perform semi-micro qualitative analysis for identifying cations and anions

COURSE CONTENT

Unit I: s- and p-Block Elements:

Periodicity in s- and p-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electronegativity (Pauling, Mulliken, and Alfred-Rochow scales). Allotropy in C, S, and P.

Oxidation states with reference to elements in unusual and rare oxidation states like carbides and nitrides), inert pair effect, diagonal relationship and anomalous behaviour of first member of each group.

Unit II: Compounds of s- and p-Block Elements

Hydrides and their classification (ionic, covalent and interstitial), structure and properties with respect to stability of hydrides of p- block elements.

Concept of multicentre bonding (diborane).

Structure, bonding and their important properties like oxidation/reduction, acidic/basic nature of the following compounds and their applications in industrial, organic and environmental chemistry.

Hydrides of nitrogen (NH_3, N_2H_4, N_3H, NH_2OH)

Oxoacids of P, S and Cl.

Halides and oxohalides: PCl_3, PCl_5, $SOCl_2$ and SO_2Cl_2

Unit III: General Principles of Metallurgy:

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon as reducing agent. Hydrometallurgy, Methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn): electrolytic, oxidative refining, Kroll process, Parting process, van Arkel-de Boer process and Mond's process.

Unit IV: Laboratory Experiments

Semi-micro qualitative analysis using H_2S of mixtures- not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

Cations: NH_4^+, Pb^{2+}, Ag^+, Bi^{3+}, Cu^{2+}, Cd^{2+}, Sn^{2+}, Fe^{3+}, Al^{3+}, Co^{2+}, Cr^{3+}, Ni^{2+}, Mn^{2+}, Zn^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+} and K^+.

Anions: CO_3^{2-}, S^{2-}, SO_2^-, $S_2O_3^{2-}$, NO_3^-, CH_3COO^-, Cl^-, Br^-, I^-, NO_3^-, SO_4^{2-}, PO_4^{3-}, BO_3^{3-}, $C_2O_4^{2-}$ and F^-

(Spot tests should be carried out wherever feasible)

Suggested Readings

[] J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry* Cengage Lening India Pvt. Ltd. (2009).
[2] B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).
[3] R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
[4] J. D. Lee: *A New Concise Inorganic Chemistry*, E.L.B.S.
[5] F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
[6] D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
[7] Gary Wulfsberg: *Inorganic Chemistry*, Viva Books Pvt. Ltd.
[8] A.I. Vogel, *Qualitative Inorganic Analysis*, Prentice Hall, 7th Edn.
[9] A.I. Vogel, *Quantitative Chemical Analysis*, Prentice Hall, 6th Edn.

Generic Elective Course: 04 Credits

CYG-106: States of Matter and Chemical Kinetics

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the kinetic theory of gases, surface tension and viscosity of liquids.
[CO.2] To know and understand the chemical kinetics including the concepts of the reaction rates and the theories of reaction rates
[CO.3] To learn how to measure the surface tension and viscosity of liquids
[CO.4] To learn how to study the kinetics of the chemical reactions

Course Outcomes:

After completion of this course,
[CO.1] Student(s) will understand the kinetic theory of gases, surface tension and viscosity of liquids.
[CO.2] Student(s) will know and understand the chemical kinetics including the concepts of the reaction rates and the theories of reaction rates
[CO.3] Student(s) will have the skills to measure the surface tension and viscosity of liquids
[CO.4] Student(s) will have the skills to study the kinetics of the chemical reactions

COURSE CONTENT

Unit I: Kinetic Theory of Gases

Postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation.

Deviation of real gases from ideal behaviour, compressibility factor, causes of deviation. van der Waals equation of state for real gases. Boyle temperature (derivation not required). Critical phenomena, critical constants and their calculation from van der Waals equation.
Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation – derivation not required) and their importance.

Temperature dependence of these distributions. Most probable, average and root mean square velocities (no derivation). Collision cross section, collision number, collision frequency, collision diameter and mean free path of molecules. Viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only).

Unit II: Liquids

Surface tension and its determination using stalagmometer. Viscosity of a liquid and determination of coefficient of viscosity using Ostwald viscometer. Effect of temperature on surface tension and coefficient of viscosity of a liquid (qualitative treatment only)

Unit III: Solids

Forms of solids. Symmetry elements, unit cells, crystal systems, Bravais lattice types and identification of lattice planes.. Miller indices. X–Ray diffraction by crystals, Bragg's law. Structures of NaCl, KCl and CsCl (qualitative treatment only). Defects in crystals. Glasses and liquid crystals.

Unit IV: Chemical Kinetics

The concept of reaction rates. Effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction. Derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants). Half–life of a reaction.

General methods for determination of order of a reaction. Concept of activation energy and its calculation from Arrhenius equation.

Theories of Reaction Rates: Collision theory and Activated Complex theory of bimolecular reactions. Comparison of the two theories (qualitative treatment only).

Unit V: Laboratory Experiments

[1] To determine the surface tension of a liquid or a dilute solution using a stalagmometer.
[2] To study the variation of surface tension of a detergent solution with concentration.
[3] To determine the relative and absolute viscosity of a liquid or dilute solution using an Ostwald's viscometer.
[4] To study the variation of viscosity of an aqueous solution with concentration of solute.
[5] To study the kinetics of the iodide-persulphate reaction using initial rate method.
[6] To study the kinetics of acid hydrolysis of methyl acetate (with hydrochloric acid) using the integrated rate method.
[7] To study of the kinetics of saponification of ethyl acetate using the integrated rate method.
[8] To compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate.

Suggested Readings

[1] G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).
[2] G. W. Castellan: *Physical Chemistry* 4th Edn. Narosa (2004).
[3] J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry* Cengage Lening India Pvt. Ltd., New Delhi (2009).
[4] B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).
[5] R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
[6] J. D. Lee: *A New Concise Inorganic Chemistry*, E.L.B.S.
[7] F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
[8] D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
[9] Gary Wulfsberg: *Inorganic Chemistry*, Viva Books Pvt. Ltd.

Generic Elective Course: 04 Credits

CYG-107: Chemistry of d-Block Elements

(*Non-Semester Specific*)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the properties of transition elements of 3d series as well as lanthanoids and actinoids

[CO.2] To know and understand the coordination chemistry with examples of the metals e.g., chromium, iron, cobalt, nickel and copper

[CO.3] To know and understand the crystal field theory and Jahn Teller distortion

[CO.4] To learn how to estimate the quantity of nickel present in a given solution as bis(dimethylglyoximato)nickel(II) or aluminium as oxinate in a given solution gravimetrically.

[CO.5] To learn how to carry out the estimation of (i) Mg^{2+} or (ii) Zn^{2+} by complexometric titrations using EDTA.

[CO.6] To learn how to estimate total hardness of a given sample of water by complexometric titration.

Course Outcomes:

After completion of this course,

[CO.1] The students will know and understand the properties of transition elements of 3d series as well as lanthanoids and actinoids

[CO.2] The students will know and understand the coordination chemistry (with examples of the metals e.g., chromium, iron, cobalt, nickel and copper), crystal field theory and Jahn Teller distortion.

[CO.3] The students will have the skills to estimate the quantity of nickel present in a given solution as bis(dimethylglyoximato)nickel(II) or aluminium as oxinate in a given solution gravimetrically.

[CO.4] The students will have the skills to carry out the estimation of (i) Mg^{2+} or (ii) Zn^{2+} by complexometric titrations using EDTA.

[CO.5] The students will have the skills to estimate total hardness of a given sample of water by complexometric titration.

COURSE CONTENT

Unit I: Transition Elements (3d series)

General group trends with special reference to electronic configuration, variable valency, colour, magnetic and catalytic properties, ability to form complexes and stability of various oxidation states (Latimer diagrams) for Mn, Fe and Cu.

Lanthanoids and actinoids: Electronic configurations, oxidation states, colour, magnetic properties, lanthanide contraction, separation of lanthanides (ion exchange method only).

Unit II: Coordination Chemistry

Valence Bond Theory (VBT): Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Structural and stereoisomerism in complexes with coordination numbers 4 and 6.

Drawbacks of VBT. IUPAC system of nomenclature.

Unit III: Crystal Field Theory

Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors affecting the magnitude of D. Spectrochemical series. Comparison of CFSE for Oh and Td complexes, Tetragonal distortion of octahedral geometry. Jahn-Teller distortion, Square planar coordination.

Unit IV: Laboratory Experiments

[1] To estimate the quantity of nickel present in a given solution as bis(dimethylglyoximato)nickel(II) or aluminium as oxinate in a given solution gravimetrically.

[2] To estimate the quantity of (i) Mg^{2+} or (ii) Zn^{2+} by complexometric titrations using EDTA.

[3] To estimate total hardness of a given sample of water by complexometric titration.

Suggested Readings

[1] J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry*, Cengage Lening India Pvt. Ltd. (2009).
[2] B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).
[3] R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
[4] J. D. Lee: *A New Concise Inorganic Chemistry*, E.L.B.S.
[5] F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
[6] D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
[7] Gary Wulfsberg: *Inorganic Chemistry*, Viva Books Pvt. Ltd.

Generic Elective Course: 04 Credits

CYG-108: Spectroscopy and Photochemistry

(*Non-Semester Specific*)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the electronic spectroscopy and photochemistry

[CO.2] To learn how to draw calibration curve (absorbance at λ_{max} vs. concentration) and use it in quantitative analysis.

[CO.3] To learn how to apply Job's method for determining the composition of the Fe^{3+} - salicylic acid complex / Fe^{2+} - phenanthroline complex in solution.

[CO.4] To learn how to use Flame Photometry for determining the concentration of Na^+ and K^+.

[CO.5] To learn how to record the UV spectra of the compounds and identify the effect of structure on the spectra.

[CO.6] To To learn how to calculate the energies of the electronic transitions in $KMnO_4$ and $K_2Cr_2O_7$ with help of values of λ_{max} in absorbance spectra.

[CO.7] To learn how to study the pH-dependence of the UV-Vis spectrum of $K_2Cr_2O_7$.

[CO.8] To learn how to verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration

[CO.9] To analyse the given vibration-rotation spectrum of HCl(g).

Course Outcomes:

After completion of this course,

[CO.1] The students will know and understand the electronic spectroscopy and photochemistry

[CO.2] The students will have the skills to draw calibration curve (absorbance at λ_{max} vs. concentration) and use it in quantitative analysis.

[CO.3] The students will have the skills to apply Job's method for determining the composition of the Fe^{3+} - salicylic acid complex / Fe^{2+} - phenanthroline complex in solution.

[CO.4] The students will have the skills to use Flame Photometry for determining the concentration of Na^+ and K^+.

[CO.5] The students will have the skills to record the UV spectra of the compounds and identify the effect of structure on the spectra.

[CO.6] The students will have the skills to learn how to calculate the energies of the electronic transitions with help of values of λ_{max} in absorbance spectra.

[CO.7] The students will have the skills to study the pH-dependence of the UV-Vis spectrum.

[CO.8] The students will have the skills to verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration

[CO.9] The students will have the skills to analyse the given vibration-rotation spectrum of HCl(g).

COURSE CONTENT

Unit I: Spectroscopy

Microwave (pure rotational) spectra of diatomic molecules. Selection rules. Structural information derived from rotational spectroscopy.

Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels. Selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies. Effect of hydrogen bonding (inter- and intramolecular) and substitution on vibrational frequencies.

Electronic Spectroscopy: Electronic excited states. Free Electron model and its application to electronic spectra of polyenes. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts.

Unit II: Photochemistry

Laws of photochemistry. Lambert-Beer's law. Fluorescence and phosphorescence. Quantum efficiency and reasons for high and low quantum yields. Primary and secondary processes in photochemical reactions. Photochemical and thermal reactions. Photoelectric cells.

Unit III: Laboratory Experiments

[1] To draw calibration curve (absorbance at λ_{max} vs. concentration) for various concentrations of a given coloured compound and estimate the concentration of the same in a given solution.

[2] To carry out the determination of the composition of the Fe^{3+} - salicylic acid complex / Fe^{2+} - phenanthroline complex in solution by Job's method.

[3] To carry out the determination of concentration of Na^+ and K^+ using Flame Photometry.

[4] To study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1} eV).

[5] To study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.

[6] To record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

[7] To verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration

[8] To analyse the given vibration-rotation spectrum of HCl(g)

Suggested Readings

[1] A.I. Vogel, *Qualitative Inorganic Analysis*, Prentice Hall, 7th Edn.

[2] A.I. Vogel, *Quantitative Chemical Analysis*, Prentice Hall, 6th Edn. • B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

[3] G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).

[4] G. W. Castellan: *Physical Chemistry* 4th Edn. Narosa (2004).

[5] J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry*, Cengage Lening India Pvt. Ltd., New Delhi (2009).

[6] B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).

[7] R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).

[8] J. D. Lee: *A New Concise Inorganic Chemistry*, E.L.B.S.

[9] F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.

[10] D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.

[11] Gary Wulfsberg: *Inorganic Chemistry*, Viva Books Pvt. Ltd.

Generic Elective Course: 04 Credits

CYG-109: Molecules of Life

(*Non-Semester Specific*)

Type	:	Elective Course
Total Credits	:	04 (Theory: 04 + Practical: 0)
Total Hours	:	60 Theory
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the classification, properties and structure of carbohydrates
[CO.2] To know and understand the amino acids, peptides and proteins
[CO.3] To know and understand the enzymes and their correlation with drug design
[CO.4] To know and understand the nucleic acids, genetic code, biological roles of DNA and RNA, replication, transcription and translation
[CO.5] To know and understand the lipids, their classification and biological importance

Course Outcomes:

After completion of the course,
[CO.1] The students will know and understand the classification, properties and structure of carbohydrates, amino acids, peptides and proteins
[CO.2] The students will know and understand the enzymes and their correlation with drug design
[CO.3] The students will know and understand the nucleic acids, genetic code, biological roles of DNA and RNA, replication, transcription and translation
[CO.4] The students will understand the lipids, their classification and biological importance

COURSE CONTENT

Unit 1: Carbohydrates

Classification of carbohydrates, reducing and non-reducing sugars, General Properties of Glucose and Fructose, their open chain structure. Epimers, mutarotation and anomers. Determination of configuration of Glucose (Fischer proof). Cyclic structure of glucose. Haworth projections.
Cyclic structure of fructose. Linkage between monosachharides, structure of disacharrides (sucrose, maltose, lactose) and polysacharrides (starch and cellulose) excluding their structure elucidation.

Unit 2: Amino Acids, Peptides and Proteins

Classification of Amino Acids, Zwitterion structure and Isoelectric point. Overview of Primary, Secondary, Tertiary and Quaternary structure of proteins. Determination of primary structure of peptides, determination of N-terminal amino acid (by DNFB and Edman method) and C-terminal amino acid (by thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) & C-activating groups and Merrifield solid phase synthesis.

Unit 3: Enzymes and correlation with drug action

Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, Specificity of enzyme action (Including stereospecifity), Enzyme inhibitors and their importance, phenomenon of inhibition (Competitive and Non-competitive inhibition including allosteric inhibtion). Drug action-receptor theory. Structure –activity relationships of drug molecules, binding role of −OH group, $-NH_2$ group, double bond and aromatic ring,

Unit 4: Nucleic Acids

Components of Nucleic acids: Adenine, guanine, thymine and Cytosine (Structure only), other components of nucleic acids, Nucleosides and nucleotides (nomenclature), Structure of

polynucleotides; Structure of DNA (Watson-Crick model) and RNA (types of RNA), Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation.

Unit 5: Lipids

Introduction to lipids, classification. Oils and fats: Common fatty acids present in oils and fats, Omega fatty acids, Trans fats, Hydrogenation, Saponification value, Iodine number. Biological importance of triglycerides, phospholipids, glycolipids, and steroids (cholesterol).

Suggested Readings:

[1] Nelson, D. L. & Cox, M. M. Lehninger's *Principles of Biochemistry* 7th Ed.

Generic Elective Course: 04 Credits

CYG-110: Energy in Biosystem and Biochemistry Lab

(*Non-Semester* Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 02 + Practical: 02)
Total Hours	:	30 Theory + 60 Practical
Lectures	:	02 per week
Tutorial	:	0
Practical	:	02 per week

Course Objectives:

[CO.1] To know and understand the concepts of the energy in biosystem, calorific value of food, oxidation of food, catabolism, anabolism, ATP, ATP hydrolysis, and catabolic pathways of carbohydrate, fats and proteins

[CO.2] To learn how to separate amino acids by paper chromatography, determine the concentration of glycine solution by formylation method, and study the titration curve of glycine

[CO.3] To learn how to study the action of salivary amylase on starch, and the effect of temperature on the action of salivary amylase on starch.

[CO.4] To learn how to determine the saponification value of an oil/fat.

[CO.5] To learn how to determine the iodine value of an oil/fat.

[CO.6] To learn how to differentiate between a reducing/ nonreducing sugar.

[CO.7] To learn how to extraction of DNA from onion/cauliflower.

[CO.8] To learn how to synthesise aspirin by acetylation of salicylic acid and compare it with the ingredient of an aspirin tablet by TLC.

Course Outcomes:

After completion of the course,

[CO.1] The student(s) will know and understand the concepts of the energy in biosystem, calorific value of food, oxidation of food, catabolism, anabolism, ATP, ATP hydrolysis, and catabolic pathways of carbohydrate, fats and proteins.

[CO.2] Learners will attain the skills to separate amino acids by paper chromatography, determine the concentration of glycine solution by formylation method, and study the titration curve of glycine.

[CO.3] Learners will acquire the skills to study the action of salivary amylase on starch, and the effect of temperature on the action of salivary amylase on starch.

[CO.4] Learners will acquire the skills to determine the saponification value of an oil/fat.

[CO.5] Learners will acquire the skills to determine the iodine value of an oil/fat.

[CO.6] Learners will have the skills to differentiate between a reducing/ nonreducing sugar.

[CO.7] Students will have the skills to extract DNA from onion/cauliflower.

[CO.8] Students will have the skills to synthesise aspirin and use TLC to compare it with the ingredient of an aspirin tablet.

COURSE CONTENT

Unit I: Concept of Energy in Biosystems

Calorific value of food. Standard caloric content of carbohydrates, proteins and fats.

Oxidation of foodstuff (organic molecules) as a source of energy for cells. Introduction to Metabolism (catabolism, anabolism),

ATP: the universal currency of cellular energy, ATP hydrolysis and free energy change.

Conversion of food into energy. Outline of catabolic pathways of Carbohydrate- Glycolysis, Fermentation, Krebs Cycle. Overview of catabolic pathways of Fats and Proteins. Interrelationships in the metabolic pathways of Proteins, Fats and Carbohydrates.

Unit II: Laboratory Experiments

[1] To separate amino acids by paper chromatography

[2] To determine the concentration of glycine solution by formylation method.
[3] To study of titration curve of glycine
[4] To study action of salivary amylase on starch
[5] To study the effect of temperature on the action of salivary amylase on starch.
[6] To determine the saponification value of an oil/fat.
[7] To determine the iodine value of an oil/fat
[8] To differentiate between a reducing/ nonreducing sugar.
[9] To extract DNA from onion/cauliflower
[10] To synthesise aspirin by acetylation of salicylic acid and compare it with the ingredient of an aspirin tablet by TLC.

Suggested Readings

[1] Nelson, D. L. & Cox, M. M. Lehninger's *Principles of Biochemistry* 7th Ed.

[2] Furniss, B.S.; Hannaford, A.J.; Rogers, V.; Smith, P.W.G.; Tatchell, A.R. Vogel's *Textbook of Practical Organic Chemistry*, ELBS.

[3] Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press.

Generic Elective Course: 04 Credits

CYG-111: Organometallics and Inorganic Synthesis

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 02 + Practical: 02)
Total Hours	:	30 Theory + 60 Practical
Lectures	:	02 per week
Tutorial	:	0
Practical	:	02 per week

Course Objectives:

[CO.1] To know and understand the chemistry of transition metals of 3d series

[CO.2] To know and understand the definition and classification of organometallic compounds, structural aspects of methyl lithium, Zeiss salt and ferrocene

[CO.3] To know and understand the preparation, structure, properties and bonding of mononuclear and polynuclear metal carbonyls of 3d series

[CO.4] To learn how to separate the mixtures of inorganic ions using paper chromatographic techniques and measure the *Rf* value

[CO.5] To learn how to prepare and synthesize inorganic coordination compounds [*such as tetraamminecarbonatocobalt (III) nitrate, tetraamminecopper (II) sulphate and potassium trioxalatoferrate (III) trihydrate*], and measure their conductivity.

Course Objectives:

After completion of the course,

[CO.1] The student(s) will know and understand the chemistry of transition metals of 3d series.

[CO.2] The student(s) will know and understand the definition and classification of organometallic compounds, structural aspects of methyl lithium, Zeiss salt and ferrocene.

[CO.3] The student(s) will know and understand the preparation, structure, properties and bonding of mononuclear and polynuclear metal carbonyls of 3d series.

[CO.4] The student(s) will have the skills to separate the mixtures of inorganic ions using paper chromatographic techniques and measure the *Rf* value

[CO.5] The student(s) will have the skills to prepare and synthesize inorganic coordination compounds [*such as tetraamminecarbonatocobalt (III) nitrate, tetraamminecopper (II) sulphate and potassium trioxalatoferrate (III) trihydrate*], and measure their conductivity.

COURSE CONTENT

Unit I: Chemistry of 3d metals

Oxidation states displayed by Cr, Fe, Co, Ni and Co.

A study of the following compounds (including preparation and important properties);

Peroxo compounds of Cr, $K_2Cr_2O_7$, $KMnO_4$, $K_4[Fe(CN)_6]$, sodium nitroprusside, $[Co(NH_3)_6]Cl_3$, $Na_3[Co(NO_2)_6]$.

Unit II: Organometallic Compounds

Definition and classification of organometallic compounds on the basis of bond type.

Concept of hapticity of organic ligands.

Metal Carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π-acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

Zeise's Salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler – Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium.

Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

Unit III: Catalysis by Organometallic Compounds

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinsons Catalyst)
2. Hydroformylation (Co salts)
3. Wacker Process
4. Synthetic gasoline (Fischer Tropsch reaction)
5. Synthesis gas by metal carbonyl complexes

Unit IV: Laboratory Experiments

[1] To separate the mixtures by paper chromatography, and measure the *Rf* value in given mixture of (Fe^{3+}, $A1^{3+}$ and Cr^{3+}) or (Ni^{2+}, Co^{2+}) or (Mn^{2+} and Zn^{2+})

[2] To prepare any two of the following complexes and measurement of their conductivity:

(i) tetraamminecarbonatocobalt (III) nitrate
(ii) tetraamminecopper (II) sulphate
(iii) potassium trioxalatoferrate (III) trihydrate

Compare the conductance of the complexes with that of M/1000 solution of NaCl, $MgCl_2$ and $LiCl_3$.

Suggested Readings

[1] James E. Huheey, Ellen Keiter & Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
[2] G.L. Miessler & Donald A. Tarr: *Inorganic Chemistry*, Pearson Publication.
[3] John R. Dyer: *Applications of Absorption Spectroscopy of Organic Compounds*, Prentice Hall.
[4] A.I. Vogel: *Qualitative Inorganic Analysis*, Prentice Hall, 7th Edn.
[5] A.I. Vogel: *Quantitative Chemical Analysis*, Prentice Hall, 6th Edn.
[6] A.I. Vogel: *Textbook of Practical Organic Chemistry*, Prentice Hall, 5th Edn.
[7] F. G. Mann & B. C. Saunders: *Practical Organic Chemistry*, Orient Longman (1960).

Generic Elective Course: 04 Credits

CYG-112: Organic Spectroscopic and Spectrometric Techniques

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

Course Objectives:

[CO.1] To be able to understand the fundamentals of UV-Vis, IR and NMR spectroscopy, interpret the data of UV-Vis, IR and NMR spectroscopic techniques in qualitative analysis and structural elucidation of organic compounds

[CO.2] To be able to elucidate the structures of organic compounds using the spectra obtained from UV-Vis, IR and NMR spectroscopic and mass spectrometric techniques.

Course Outcomes:

After completing the course,

[CO.1] The students will be able to understand the fundamentals of UV-Vis, IR and NMR spectroscopy, and interpret the data of UV-Vis, IR and NMR spectroscopic techniques in qualitative analysis and structural elucidation of organic compounds.

[CLO.1] The students will be able to elucidate the structures of organic compounds using the spectra obtained from UV-Vis, IR and NMR spectroscopic and mass spectrometric techniques.

COURSE CONTENT

Unit I:

General principles Introduction to absorption and emission spectroscopy.

Unit II: UV Spectroscopy

Types of electronic transitions, λmax, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of λ_{max} for the following systems: α, β unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); distinction between *cis*- and *trans*-isomers.

Unit III: IR Spectroscopy

Fundamental and non-fundamental molecular vibrations; IR absorption positions of O, N and S containing functional groups; Effect of H-bonding, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis.

Unit IV: NMR Spectroscopy

Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin – Spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Hydrogen deficiency index (HDI) or Index of unsaturation, Interpetation of NMR spectra of simple compounds.

Unit V: Mass Spectrometry

Mass spectrometry and its usefulness, Basic components and Functions of Mass Spectrometer, Mass Spectrum: molecular ion(s), and formation of fragments, molecular ion peak, base peak, radical cation, fragment ions, m/z ratio. Resolution, Atomic weight, Average mass, Monoisotopic mass, Exact mass, Nominal mass, Relative atomic mass, Use of mass spectral data in determining average relative atomic mass as well as relative molecular mass, application of high resolution mass spectrometry (HRMS) in the determination of molecular formula, Nitrogen rule, The rule of thirteen, Fragmentation patterns of

straight chain alkanes, Stevenson's rule, branched chain alkanes, alkenes, cycloalkenes, alkynes, aromatic hydrocarbons, alkyl-substituted aromatic hydrocarbons, aldehydes, ketones, Mc-Lafferty rearrangement, esters, carboxylic acids, amides, alcohols, phenols, ethers, haloalkanes, haloarenes, amines, nitriles and organic nitro compounds. Examples of mass spectrum of rubidium, lead, Cl_2, chloromethane, dichloromethane, straight chain alkanes, branched alkanes, cycloalkanes, alkenes, cycloalkenes, alkynes, aromatic hydrocarbons and their derivatives, aldehydes and ketones, esters, aliphatic carboxylic acids, aromatic carboxylic acids, amides, alcohols, phenols, aliphatic ethers, aromatic ethers, alkyl halides, aryl halides, amines, alkyl nitriles, nitro compounds and other simple organic molecules.

Unit VI:

Applications of IR, UV and NMR spectroscopic and mass spectrometric data for identification of simple organic molecules.

Suggested Readings

[1] P.S. Kalsi, "*Spectroscopy of Organic Compounds*" 9th Edition (2022), New Age Publishers.
[2] Jiben Roy, "*A Self-Study Guide to the Principles of Organic Chemistry*" Universal Publishers.
[3] Silverstein, R. M., Webseter, F. X. and Kiemle, D., *"Spectrometric Identification of Organic Compounds"*, 7th Ed., John Wiley &Sons.
[4] Kemp, W. L., *"Organic Spectroscopy"*, Palgrave.
[5] Pavia, D. L., *"Spectroscopy"*,4th Ed., Cengage.
[6] Williams, D. and Fleming, l., *"Spectroscopic Methods in Organic Chemistry"*, 6th Ed., McGraw Hill Education (India) Private Limited.

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Generic Elective Course: 04 Credits

CYG-113: Bioinorganic Chemistry and Polynuclear Hydrocarbons

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the bioinorganic chemistry, role of metal ions in biological systems
[CO.2] To know and understand the polynuclear and heteronuclear hydrocarbons
[CO.3] To know and understand the active methylene compounds and their reactions
[CO.4] To learn how to carry out the systematic qualitative organic analysis of organic compounds possessing monofunctional groups (-COOH, phenolic, aldehydic, ketonic, amide, nitro, amines) and preparation of one derivative.

Course Outcomes:

After completion of this course,
[CO.1] The student(s) will know and understand the bioinorganic chemistry, role of metal ions in biological systems.
[CO.2] The student(s) will know and understand the polynuclear and heteronuclear hydrocarbons.
[CO.3] The student(s) will know and understand the active methylene compounds and their reactions.
[CO.4] The student(s) will have the skills to carry out the systematic qualitative organic analysis of organic compounds possessing monofunctional groups (-COOH, phenolic, aldehydic, ketonic, amide, nitro, amines) and preparation of one derivative.

COURSE CONTENT

Unit I: Bio-Inorganic Chemistry

A brief introduction to bio-inorganic chemistry. Role of metal ions present in biological systems with special reference to Na^+, K^+ and Mg^{2+} ions: Na/K pump; Role of Mg^{2+} ions in energy production and chlorophyll. Role of Ca^{2+} in blood clotting, stabilization of protein structures and structural role (bones).

Unit II: Polynuclear and heteronuclear aromatic compounds:

Properties of the following compounds with reference to electrophilic and nucleophilic substitution: Naphthalene, Anthracene, Furan, Pyrrole, Thiophene, and Pyridine.

Unit III: Active methylene compounds:

Preparation: Claisen ester condensation. Keto-enol tautomerism.
Reactions: Synthetic uses of ethylacetoacetate (preparation of non-heteromolecules having upto 6 carbon).

Unit IV: Laboratory Experiments

Systematic qualitative organic analysis of organic compounds possessing monofunctional groups (-COOH, phenolic, aldehydic, ketonic, amide, nitro, amines) and preparation of one derivative.

Suggested Readings

[1] James E. Huheey, Ellen Keiter & Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
[2] G.L. Miessler & Donald A. Tarr: *Inorganic Chemistry*, Pearson Publication.
[3] John R. Dyer: *Applications of Absorption Spectroscopy of Organic Compounds*, Prentice Hall.
[4] A.I. Vogel: *Qualitative Inorganic Analysis*, Prentice Hall, 7th Edn.
[5] A.I. Vogel: *Quantitative Chemical Analysis*, Prentice Hall, 6th Edn.
[6] A.I. Vogel: *Textbook of Practical Organic Chemistry*, Prentice Hall, 5th Edn.
[7] F. G. Mann & B. C. Saunders: *Practical Organic Chemistry*, Orient Longman (1960).

Generic Elective Course: 04 Credits

CYG-114: Phase Equilibrium, Conductance and Electrochemistry

(*Non-Semester Specific*)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the concepts of solutions, phase equilibrium, conductance and electrochemistry

[CO.2] To learn how to construct the phase diagram of a binary system (simple eutectic) using cooling curves.

[CO.2] To learn how to determine the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.

[CO.3] To learn how to carry out the experiments in the laboratory to determine cell constant, equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

[CO.4] To learn how to perform the experiments in the laboratory to carry out conductometric titrations.

Course Outcomes:

After completion of this course,

[CO.1] The student(s) will know and understand the concepts of solutions, phase equilibrium, conductance and electrochemistry

[CO.2] The student(s) will have the skills to construct the phase diagram of a binary system (simple eutectic) using cooling curves.

[CO.3] The student(s) will have the skills to determine the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.

[CO.4] The student(s) will have the skills to carry out the experiments in the laboratory to determine cell constant, equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

[CO.5] The student(s) will have the skills to perform the experiments in the laboratory to carry out conductometric titrations.

COURSE CONTENT

Unit I: Phase Equilibrium

Phases, components and degrees of freedom of a system, criteria of phase equilibrium. Gibbs Phase Rule and its thermodynamic derivation. Derivation of Clausius – Clapeyron equation and its importance in phase equilibria. Phase diagrams of one-component systems (water and sulphur) and two component systems involving eutectics, congruent and incongruent melting points (lead-silver, $FeCl_3$-H_2O and Na-K only).

Unit II: Conductance

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch law of independent migration of ions. Transference number and its experimental determination using Hittorf and Moving boundary methods. Ionic mobility. Applications of conductance measurements: determination of degree of ionization of weak electrolyte, solubility and solubility products of sparingly soluble salts, ionic product of water, hydrolysis constant of a salt. Conductometric titrations (only acid-base).

Unit III: Electrochemistry

Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell. Nernst equation and its importance. Types of electrodes. Standard electrode potential. Electrochemical series.

Thermodynamics of a reversible cell, calculation of thermodynamic properties: ΔG, ΔH and ΔS from EMF data.

Calculation of equilibrium constant from EMF data. Concentration cells with transference and without transference. Liquid junction potential and salt bridge.

pH determination using hydrogen electrode and quinhydrone electrode.

Potentiometric titrations -qualitative treatment (acid-base and oxidation-reduction only).

Unit IV: Laboratory Experiments

[1] To study the equilibrium of one of the following reactions by the distribution method:

$I_2(aq) + I^-(aq) \rightleftharpoons I_3^-(aq)$

$Cu^{2+}(aq) + xNH_2(aq) \rightleftharpoons [Cu(NH_3)_x]^{2+}$

[2] To construct the phase diagram of a binary system (simple eutectic) using cooling curves.

[3] To determine the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.

[4] To study the variation of mutual solubility temperature with concentration for the phenol water system and determination of the critical solubility temperature.

[5] To determine the cell constant

[6] To determine equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

[7] To perform the conductometric titrations:

[i] Strong acid *versus* strong base

(ii) Weak acid *versus* strong base

[8] To perform the following potentiometric titrations:

[i] Strong acid vs. strong base

[ii] Weak acid vs. strong base

[iii] Potassium dichromate vs. Mohr's salt

Suggested Readings

[1] G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).

[2] G. W. Castellan: *Physical Chemistry* 4th Ed. Narosa (2004).

[3] J. C. Kotz, P. M. Treichel, J. R. Townsend, *General Chemistry*, Cengage Learning India Pvt. Ltd.: New Delhi (2009).

[4] B. H. Mahan: *University Chemistry*, 3rd Edn. Narosa (1998).

[5] R. H. Petrucci, *General Chemistry*, 5th Edn., Macmillan Publishing Co.: New York (1985).

[6] B.D. Khosla: *Senior Practical Physical Chemistry*, R. Chand & Co.

Generic Elective Course: 04 Credits

CYG-115: Carboxylic Acids, Amines and Derivatives

(*Non-Semester Specific*)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the methods of preparation and chemical properties of carboxylic acids, derivatives of carboxylic acids, amines and diazonium salts

[CO.2] To know and understand the methods of preparation and properties of amino acids, peptides and proteins

Course Outcomes:

After completion of this course,

[CO.1] The student(s) will know and understand the methods of preparation and chemical properties of carboxylic acids, derivatives of carboxylic acids, amines and diazonium salts

[CO.2] The student(s) will know and understand the methods of preparation and properties of amino acids, peptides and proteins

COURSE CONTENT

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

Unit I: Carboxylic acids and their derivatives

Carboxylic acids (aliphatic and aromatic):

Preparation: Acidic and Alkaline hydrolysis of esters.

Reactions: Hell – Vohlard - Zelinsky Reaction.

Unit II: Carboxylic acid derivatives (aliphatic): (Upto 5 carbons)

Preparation: Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversion.

Reactions: Comparative study of nucleophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation.

Unit III: Amines and Diazonium Salts

Amines (Aliphatic and Aromatic): (Upto 5 carbons)

Preparation: from alkyl halides, Gabriel's Phthalimide synthesis, Hofmann Bromamide reaction.

Reactions: Hofmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, with HNO_2, Schotten – Baumann Reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation.

Diazonium salts:

Preparation: from aromatic amines.

Reactions: conversion to benzene, phenol, dyes.

Unit IV: Amino Acids, Peptides and Proteins

Preparation of Amino Acids: Strecker synthesis using Gabriel's phthalimide synthesis. Zwitterion, Isoelectric point and Electrophoresis.

Reactions of Amino acids: ester of –COOH group, acetylation of $–NH_2$ group, complexation with Cu^{2+} ions, ninhydrin test.

Overview of Primary, Secondary, Tertiary and Quaternary Structure of proteins.

Determination of Primary structure of Peptides by degradation Edmann degradation (N-terminal) and C-terminal (thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) & C-activating groups and Merrifield solid-phase synthesis.

Suggested Readings

[1] J. C. Kotz, P. M. Treichel, J. R. Townsend, *General Chemistry*, Cengage Learning India Pvt. Ltd.: New Delhi (2009).
[2] B. H. Mahan: *University Chemistry*, 3rd Edn. Narosa (1998).
[3] R. H. Petrucci, *General Chemistry*, 5th Edn., Macmillan Publishing Co.: New York (1985).
[4] Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
[5] Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
[6] A.I. Vogel: *Textbook of Practical Organic Chemistry*, Prentice Hall, 5th Edn.
[7] F. G. Mann & B. C. Saunders: *Practical Organic Chemistry*, Orient Longman, 1960.
[8] Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press.

Skill Enhancement Course

CYG-116: Chemistry of Fuels and Pesticides

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practicals
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To understand and know about renewable and non-renewable sources of energy, different types of fuels and their calorific values, [CO.2] To understand the uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal.
[CO.3] To understand the composition and uses of coal gas, producer gas and water gas.
[CO.4] To know about petroleum and petrochemical industry, different types of petroleum products and their applications.
[CO.5] To know about the lubricants and their classification, properties of lubricants (viscosity index, cloud point, pore point) and their determination.

Course Outcomes:

After completion of this course,
[CO.1] Student(s) will understand and know the renewable and non-renewable sources of energy, different types of fuels and their calorific values
[CO.2] Student(s) will understand and know the uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal.
[CO.3] Student(s) will understand the composition and uses of coal gas, producer gas and water gas.
[CO.4] Student(s) will know about petroleum and petrochemical industry, different types of petroleum products and their applications.
[CO.5] Student(s) will know about the lubricants and their classification, properties of lubricants (viscosity index, cloud point, pore point) and their determination.

COURSE CONTENT

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value. Gross calorific value, net calorific value, determination of calorific value using Bomb calorimeter.

Unit I: Coal

Uses of coal (fuel and nonfuel) in various industries, its composition, proximate analysis, ultimate analysis, determination of % of carbon, hydrogen, nitrogen, sulphur, ash and oxygen. Carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Unit II: Petroleum Industry

Composition of crude petroleum, Refining and different types of petroleum products, Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), knocking, octane number, unleaded petrol, Reforming, Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels.

Unit III: Lubricants

Classification of lubricants, lubricating oils (conducting and non-conducting), Solid and semisolid lubricants, synthetic lubricants. Properties of lubricants (viscosity index, cloud point, pore point, flash point, fire point) and their determination.

Unit IV: Pesticides

General introduction to pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides, structure activity relationship, synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,); Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor).

Unit V: Laboratory Experiments

[1] To calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.

[2] To prepare simple organophosphates, phosphonates and thiophosphates

Suggested Readings

[1] E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.
[2] P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
[3] B.K. Sharma: *Industrial Chemistry*, Goel Publishing House, Meerut.
[4] R. Cremlyn: *Pesticides*, John Wiley

Skill Enhancement Course

CYS-101: Fuel Chemistry

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 02 + Practical: 0)
Total Hours	:	30 Theory
Lectures	:	02 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To be able to understand Renewable and non-renewable sources of energy, different types of fuels and their calorific values

[CO.2] To understand the uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal.

[CO.3] To understand the composition and uses of coal gas, producer gas and water gas.

[CO.4] To know about petroleum and petrochemical industry, different types of petroleum products and their applications.

[CO.5] To know about the lubricants and their classification, properties of lubricants (viscosity index, cloud point, pore point) and their determination.

Course Outcomes:

After completion of this course,

[CO.1] Student(s) will understand and know the renewable and non-renewable sources of energy, different types of fuels and their calorific values.

[CO.2] Student(s) will understand and know the uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal.

[CO.3] Student(s) will understand the composition and uses of coal gas, producer gas and water gas.

[CO.4] Student(s) will know about petroleum and petrochemical industry, different types of petroleum products and their applications.

[CO.5] Student(s) will know about the lubricants and their classification, properties of lubricants (viscosity index, cloud point, pore point) and their determination.

COURSE CONTENT

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value. Gross calorific value, net calorific value, determination of calorific value using Bomb calorimeter.

Unit I: Coal

Uses of coal (fuel and nonfuel) in various industries, its composition, proximate analysis, ultimate analysis, determination of % of carbon, hydrogen, nitrogen, sulphur, ash and oxygen. Carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Unit II: Petroleum Industry

Composition of crude petroleum, Refining and different types of petroleum products, Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), knocking, octane number, unleaded petrol, Reforming, Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels.

Unit III: Lubricants

Classification of lubricants, lubricating oils (conducting and non-conducting), Solid and semisolid lubricants, synthetic lubricants. Properties of lubricants (viscosity index, cloud point, pore point, flash point, fire point) and their determination.

Suggested Readings

[1] E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.
[2] P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
[3] B.K. Sharma: *Industrial Chemistry*, Goel Publishing House, Meerut.

Skill Enhancement Course

CYS-102: Basic Organic Synthesis Lab

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 0 + Practical: 02)
Total Hours	:	00 Theory + 60 Practical
Lectures	:	0 per week
Tutorial	:	0 per week
Practical	:	2 per week

Course Objectives:

[CO.1] To learn how to carry out functional group tests

[CO.2] To learn how to carry out the organic reactions (such as acetylation, benzoylation, oxidation, reduction, hydrolysis, condensation, aldol condensation and benzil-benzilic acid rearrangement reactions), commonly used in organic synthesis.

[CO.3] To learn how to generate the nucleophile from substituted thiophenol(s) and use the same in nucleophilic substitution reaction of primary alkyl halide

Course Outcomes:

After completion of the course,

[CO.1] Student(s) will have the skills to carry out functional group tests.

[CO.2] Student(s) will have the skills to carry out the organic reactions (such as acetylation, benzoylation, oxidation, reduction, hydrolysis, condensation, aldol condensation and benzil-benzilic acid rearrangement reactions), commonly used in organic synthesis.

[CO.3] Student(s) will have the skills to generate the nucleophile from substituted thiophenol(s) and use the same in nucleophilic substitution reaction of primary alkyl halide(s).

COURSE CONTENT

[1] To perform functional group test(s) for alcohols, phenols, carbonyl and carboxylic acid group.

[2] To perform aldol condensation between acetone and benzaldehyde using either conventional or green method.

[3] To carry out benzil-benzilic acid rearrangement.

[4] To preparation of pinacolone from pinacol

[5] To perform the following reactions for preparing organic compounds:

(i) Acetylation of one of the following compounds: amines (aniline, *o*-, *m*-, *p*-toluidines, and *o*-, *m*-, *p*-anisidine) and phenols (β-naphthol, vanillin, salicylic acid) by any one method: (a) Using conventional method, (b) Using green approach

(ii) Benzolyation of one of the following amines (aniline, *o*-, *m*-, *p*- toluidines and *o*-, *m*-, *p*-anisidine) and one of the following phenols (β-naphthol, resorcinol, pcresol) by Schotten-Baumann reaction.

(iii) Oxidation of ethanol/ isopropanol (Iodoform reaction).

(iv) Bromination of any one of the following: (a) *Acetanilide by conventional methods*, (b) *Acetanilide using green approach (Bromate-bromide method)*, (c) *Nitration of any one of the following: Nitration of Acetanilide/nitrobenzene by conventional method or Nitration of Salicylic acid by green approach (using ceric ammonium nitrate)*.

(vi) Selective reduction of *meta* dinitrobenzene to *m*-nitroaniline.

(vii) Reduction of *p*-nitrobenzaldehyde by sodium borohydride.

(viii) Hydrolysis of amides and esters.

(ix) Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.

(x) *S*-Benzylisothiouronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).

Note: The above derivatives should be prepared using 0.5-1g of the organic compound. The solid samples must be collected and may be used for recrystallization, melting point and TLC.

[3] To generate nucleophile from substituted thiophenol(s) and use the same in nucleophilic substitution reaction of primary alkyl halide(s)

Suggested Readings

[1] Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry,* Pearson Education (2009)
[2] Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012)
[3] Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis,* University Press (2000).
[4] Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis,* University Press (2000).

Skill Enhancement Course

CYS-103: Pesticide Chemistry

(Non-Semester Specific)

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 01 + Practical: 01)
Total Hours	:	15 Theory + 30 Practical
Lectures	:	01 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To be able to understand the pesticides (natural and synthetic) and their benefits and adverse effects.
[CO.2] To understand changing concepts of pesticides and structure activity relationship.
[CO.3] To understand the synthesis and technical manufacturing of (i) DDT i.e., gammaxene (ii) malathion, carbofuran and carbaryl, chloranil, alachlor and butachlor.
[CO.4] To learn how to perform experiments in the laboratory to calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
[CO.5] To learn how to synthesize and prepare simple organophosphates, phosphonates and thiophosphates in laboratory.

Course Outcomes:

After completion of this course,
[CO.1] Student(s) will know and understand the pesticides (natural and synthetic) and their benefits and adverse effects.
[CO.2] Student(s) will know and understand the changing concepts of pesticides and structure activity relationship.
[CO.3] Student(s) will know and understand the synthesis and technical manufacturing of (i) DDT i.e., gammaxene (ii) malathion, carbofuran and carbaryl, chloranil, alachlor and butachlor.
[CO.4] Student(s) will have the skills to perform experiments in the laboratory to calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
[CO.5] Student(s) will have the skills to perform experiments in the laboratory to synthesize and prepare simple organophosphates, phosphonates and thiophosphates.

COURSE CONTENT

General introduction to pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides, structure activity relationship, synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,); Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor).

How to calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications. Preparation of simple organophosphates, phosphonates and thiophosphates.

Suggested Readings

[1] R. Cremlyn: Pesticides, John Wiley

Skill Enhancement Course

CYS-104: Chemistry of Cosmetics and Perfumes

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 01 + Practical: 01)
Total Hours	:	15 Theory + 30 Practical
Lectures	:	01 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To understand the methods of preparation and uses of (i) hair dye, (ii) hair spray, (iii) shampoo, (iv) suntan lotions, (v) face powder, (vi) lipsticks, (vii) talcum powder, (viii) nail enamel, (ix) creams, (x) antiperspirants and artificial flavours.

[CO.2] To know about the essential oils (such as eugenol, geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, jasmone, civetone, muscone and their importance in cosmetic industries.

[CO.3] To learn how to perform experiments in the laboratory for preparing (i) talcum powder, (ii) shampoo, (iii) enamels, (iv) hair remover, (v) face cream, and (vi) nail polish and nail polish remover.

Course Outcomes:

After completion of this course,

[CO.1] The student(s) will know and understand the methods of preparation and uses of (i) hair dye, (ii) hair spray, (iii) shampoo, (iv) suntan lotions, (v) face powder, (vi) lipsticks, (vii) talcum powder, (viii) nail enamel, (ix) creams, (x) antiperspirants and artificial flavours.

[CO.2] The student(s) will know and understand the essential oils (such as eugenol, geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, jasmone, civetone, muscone and their importance in cosmetic industries.

[CO.3] The student(s) will have the skills to perform experiments in the laboratory for preparing (i) talcum powder, (ii) shampoo, (iii) enamels, (iv) hair remover, (v) face cream, and (vi) nail polish and nail polish remover.

COURSE CONTENT

A general study including preparation and uses of the following:

Hair dye, hair spray, shampoo, suntan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone. Preparation of common cosmetic products such as talcum powder, shampoo, enamels, hair remover, face cream, nail polish and nail polish remover.

Suggested Readings

[1] E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.

[2] P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.

[3] B.K. Sharma: *Industrial Chemistry*, Goel Publishing House, Meerut.

Skill Enhancement Course

CYS-105: IT Skills for Chemists

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 01 + Practical: 01)
Total Hours	:	15 Theory + 30 Practical
Lectures	:	01 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To understand and know the fundamentals of mathematical functions, uncertainty in experimental techniques, uncertainty in measurement, statistical treatment, algebraic operations on real scalar variables, differential calculus, and numerical integration.
[CO.2] To learn how to do the computer programming
[CO.3] To learn how to use word processor and structure drawing (ChemSketch) software for the writing activities.
[CO.4] To learn how to handle data using spreadsheet software (Excel), and plot the graphs using a spreadsheet, spectral data etc.
[CO.5] To learn how to do statistical analysis

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will understand and know the fundamentals of mathematical functions, uncertainty in experimental techniques, uncertainty in measurement, statistical treatment, algebraic operations on real scalar variables, differential calculus, and numerical integration.
[CO.2] Student(s) will have the skills to do the computer programming.
[CO.3] Student(s) will have the skills to use word processor and structure drawing (ChemSketch) software for the writing activities.
[CO.4] Student(s) will have the skills to handle data using spreadsheet software (Excel), and plot the graphs using a spreadsheet, spectral data etc.
[CO.5] Student(s) will have the skills to do statistical analysis.

COURSE CONTENT

Unit I: Mathematics

Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).

Algebraic operations on real scalar variables (e.g., manipulation of van der Waals equation in different forms). Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary –bisection, e.g., pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

Numerical integration (Trapezoidal and Simpson's rule, e.g., entropy/enthalpy change from heat capacity data).

Unit II: Computer programming:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

BASIC programs for curve fitting, numerical differentiation and integration (Trapezoidal rule, Simpson's rule), finding roots (quadratic formula, iterative, Newton-Raphson method).

Unit III: HANDS ON:

Introductory writing activities:

Introduction to word processor and structure drawing (ChemSketch) software. Incorporating chemical structures, chemical equations, expressions from chemistry (e.g. Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

Handling numeric data:

Spreadsheet software (Excel), creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs. Incorporating tables and graphs into word processing documents. Simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies. Graphical solution of equations.

Numeric modelling:

Simulation of pH metric titration curves. Excel functions LINEST and Least Squares. Numerical curve fitting, linear regression (rate constants from concentration-time data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pKa of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data).

Statistical analysis:

Gaussian distribution and Errors in measurements and their effect on data sets. Descriptive statistics using Excel. Statistical significance testing: The t test. The F test.

Presentation:

Presentation graphics

Suggested Readings

[1] McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
[2] Mortimer, R. *Mathematics for Physical Chemistry*. 3 rd Ed. Elsevier (2005).
[3] Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
[4] Yates, P. *Chemical calculations*. 2 nd Ed. CRC Press (2007).
[5] Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
[6] Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
[7] Noggle, J. H. *Physical chemistry on a Microcomputer*. Little Brown & Co. (1985).
[8] Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).

Skill Enhancement Course

CYS-106: Chemical Technology and Society

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 02 + Practical: 0)
Total Hours	:	30 Theory
Lectures	:	02 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the chemical technologies for distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, and separation by absorption and adsorption.
[CO.2] To know and understand the scope of different types of equipments including reactors, distillation columns, extruders, pumps, mills, emulgators.
[CO.3] To know and learn how to scaling up the operations in chemical industry and clean technology
[CO.4] To know and understand the societal and technological issues from a chemical perspective

Course Outcomes:

After completion of this course,
[CO.1] The student(s) will understand the chemical technologies for distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, and separation by absorption and adsorption.
[CO.2] The student(s) will know and understand the scope of different types of equipments including reactors, distillation columns, extruders, pumps, mills, and emulgators.
[CO.3] The student(s) will know and learn how to scaling up the operations in chemical industry and clean technology.
[CO.4] The student(s) will know and understand the societal and technological issues from a chemical perspective.

COURSE CONTENT

Unit I: Chemical Technology

Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

Unit II: Society

Exploration of societal and technological issues from a chemical perspective. Chemical and scientific literacy as a means to better understand topics like air and water (and the trace materials found in them that are referred to as pollutants); energy from natural sources (i.e. solar and renewable forms), from fossil fuels and from nuclear fission; materials like plastics and polymers and their natural analogues, proteins and nucleic acids, and molecular reactivity and interconversions from simple examples like combustion to complex instances like genetic engineering and the manufacture of drugs.

Suggested Readings

[1] John W. Hill, Terry W. McCreary & Doris K. Kolb, *Chemistry for changing times* 13th Ed.

Skill Enhancement Course

CYS-107: Business Skills for Chemists

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 02 + Practical: 0)
Total Hours	:	30 Theory
Lectures	:	02 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To understand the basic key business concepts including business plans, market need, project management and routes to market.
[CO.2] To know about the current challenges and opportunities for the chemistry in industries.
[CO.3] To understand the role of chemistry in India and global economies.
[CO.4] To understand the financial aspects of business with case studies
[CO.5] To understand the concept of intellectual property including patents

Course Outcomes:

After completion of this course,
[CO.1] The student(s) will understand and know the basic key business concepts including business plans, market need, project management and routes to market.
[CO.2] The student(s) will understand and know the current challenges and opportunities for the chemistry in industries.
[CO.3] The student(s) will understand and know the role of chemistry in India and global economies.
[CO.4] The student(s) will understand and know the financial aspects of business with case studies.
[CO.5] The student(s) will understand and know the concept of intellectual property including patents.

COURSE CONTENT

Unit I: Business Basics

Key business concepts: Business plans, market need, project management and routes to market.

Unit II: Chemistry in Industry

Current challenges and opportunities for the chemistry-using industries, role of chemistry in India and global economies.

Unit III: Making money

Financial aspects of business with case studies

Unit IV: Intellectual property

Concept of intellectual property, patents.

Suggested Readings

www.rsc.org

Skill Enhancement Course

CYS-108: Cheminformatics

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 01 + Practical: 01)
Total Hours	:	15 Theory + 30 Practical
Lectures	:	01 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To understand and know the history, evolution, use, and prospects of chemoinformatics.
[CO.2] To understand and know molecular modelling and structure elucidation.
[CO.3] To understand and know the representation of molecules and chemical reactions.
[CO.4] To understand and know different applications of cheminformatics.

Course Outcomes:

After completion of this course,
[CO.1] Student(s) will understand the history, evolution, use, and prospects of chemoinformatics.
[CO.2] Student(s) will understand and know molecular modelling and structure elucidation.
[CO.3] Student(s) will understand and know the representation of molecules and chemical reactions.
[CO.4] Student(s) will understand and know different applications of cheminformatics.

COURSE CONTENT

Unit I: Introduction to Chemoinformatics

History and evolution of chemoinformatics, Use of chemoinformatics, Prospects of chemoinformatics, Molecular Modelling and Structure elucidation.

Unit II: Representation of molecules and chemical reactions

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Unit III: Searching chemical structures

Full structure search, sub-structure search, basic ideas, similarity search, three-dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

Unit IV: Applications

Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modeling Toxicity; Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer Assisted Structure elucidations; Computer Assisted Synthesis Design, Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design; Application of Chemoinformatics in Drug Design. Hands-on Exercises

Suggested Readings

[1] Andrew R. Leach & Valerie, J. Gillet (2007) *An introduction to Chemoinformatics*. Springer: The Netherlands.
[2] Gasteiger, J. & Engel, T. (2003) *Chemoinformatics*: A text-book. Wiley-VCH.
[3] Gupta, S. P. (2011) *QSAR & Molecular Modeling*. Anamaya Pub.: New Delhi

Skill Enhancement Course

CYS-109: Intellectual Property Rights

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 02 + Practical: 0)
Total Hours	:	30 Theory + 0 Practical
Lectures	:	01 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To understand and know the history, types and importance of intellectual property.
[CO.2] To understand and know the difference between copyrights and patents.
[CO.3] To understand and know the trademarks and their types including collective marks, certification marks, service marks, trade names, etc.
[CO.4] To understand and know the patents, geographical indications, industrial designs, trade secrets.
[CO.8] To understand and know the international agreements including (a) world trade organization (WTO) (b) Paris Convention
[CO.9] To understand and know the WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity
[CO.10] To understand and know the IP infringement issue and enforcement

Course Outcomes:

After completion of the course,
[CO.1] Students will understand the history, types and importance of intellectual property.
[CO.2] Students will understand and know the difference between copyrights and patents.
[CO.3] Students will understand and know the trademarks and their types including collective marks, certification marks, service marks, trade names, etc.
[CO.4] Students will understand and know the patents, geographical indications, industrial designs, trade secrets.
[CO.8] Students will understand and know the international agreements including (a) world trade organization (WTO) (b) Paris Convention.
[CO.9] Students will understand and know the WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity.
[CO.10] Students will understand and know the IP infringement issues and enforcement.

COURSE CONTENT

Unit I: Introduction to Intellectual Property

Historical Perspective, Different Types of IP, Importance of protecting IP.

Unit II: Copyrights

Introduction, How to obtain, Differences from Patents.

Unit III: Trade Marks

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, Trade names, etc.

Differences from Designs.

Unit IV: Patents

Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Healthcare – balancing promoting innovation with public health, Software patents and their importance for India.

Unit V: Geographical Indications

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Unit VI: Industrial Designs

Definition, How to obtain, features, International design registration.

Unit VII: Layout design of integrated circuits

Circuit Boards, Integrated Chips, Importance for electronic industry.

Unit VIII: Trade Secrets

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

Unit IX: Different International Agreements

(a) Word Trade Organization (WTO):

(i) General Agreement on Tariffs & Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement

(ii) General Agreement on Trade related Services (GATS)

(iii) Madrid Protocol

(iv) Berne Convention

(v) Budapest Treaty

(b) Paris Convention

Unit X: WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity

Unit XI: IP Infringement Issue and Enforcement

Role of Judiciary, Role of law enforcement agencies – Police, Customs etc. Economic Value of Intellectual Property – Intangible assets and their valuation, Intellectual Property in the Indian Context – Various laws in India Licensing and technology transfer.

Suggested Readings

[1] N.K. Acharya: *Textbook on intellectual property rights*, Asia Law House (2001).

[2] Manjula Guru & M.B. Rao, *Understanding Trips: Managing Knowledge in Developing Countries*, Sage Publications (2003).

[3] P. Ganguli, *Intellectual Property Rights: Unleashing the Knowledge Economy*, Tata McGraw-Hill (2001).

Skill Enhancement Course

CYS-110: Analytical Clinical Biochemistry

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 01 + Practical: 01)
Total Hours	:	15 Theory + 30 Practical
Lectures	:	01 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the structures, properties and functions of carbohydrates, proteins, enzymes, lipoproteins and DNA

[CO.2] To know and understand blood and urine analysis and to use the data and results as a diagnostic approach for correlating with biochemistry of disease

[CO.3] To learn how to carry out the qualitative and quantitative analysis in the laboratory to identify and estimate (i) carbohydrates and (ii) lipids – qualitative.

[CO.4] To learn how to determine (i) iodine number of oil, (ii) saponification number of oil, (iii) cholesterol using Liebermann- Burchard reaction

[CO.5] To learn how to carry out the qualitative analysis of proteins

[CO.6] To learn how to isolate protein, and determine it using the Biuret reaction

[CO.7] To learn how to determine the nucleic acids

Course Outcomes:

After completion of the course,

[CO.1] Students will know and understand the structures, properties and functions of carbohydrates, proteins, enzymes, lipoproteins and DNA.

[CO.2] Students will know and understand blood and urine analysis and also the use of the data and results as a diagnostic approach for correlating with biochemistry of disease.

[CO.3] Students will have the skills to carry out the qualitative and quantitative analysis in the laboratory to identify and estimate (i) carbohydrates and (ii) lipids – qualitative.

[CO.4] Students will have the skills to determine (i) iodine number of oil, (ii) saponification number of oil, (iii) cholesterol using Liebermann- Burchard reaction.

[CO.5] Students will have the skills to carry out the qualitative analysis of proteins.

[CO.6] Students will have the skills to isolate protein, and determine it using the Biuret reaction.

[CO.7] Students will have the skills to determine the nucleic acids.

COURSE CONTENT

Unit I: Basic understanding of the structures, properties and functions of carbohydrates, lipids and proteins

Review of concepts studied in the core course:

Carbohydrates: Biological importance of carbohydrates, Metabolism, Cellular currency of energy (ATP), Glycolysis, Alcoholic and Lactic acid fermentations, Krebs cycle. Isolation and characterization of polysachharides.

Proteins: Classification, biological importance; Primary and secondary and tertiary structures of proteins: α-helix and β- pleated sheets, Isolation, characterization, denaturation of proteins.

Enzymes: Nomenclature, Characteristics (mention of Ribozymes), Classification; Active site, Mechanism of enzyme action, Stereospecificity of enzymes, Coenzymes and cofactors, Enzyme inhibitors, Introduction to Biocatalysis: Importance in "Green Chemistry" and Chemical Industry.

Lipids: Classification. Biological importance of triglycerides and phosphoglycerides and cholesterol; Lipid membrane, Liposomes and their biological functions and underlying applications.

Lipoproteins.

Properties, functions and biochemical functions of steroid hormones.

Biochemistry of peptide hormones.

Structure of DNA (Watson-Crick model) and RNA, Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation, Introduction to Gene therapy.

Enzymes: Nomenclature, classification, effect of pH, temperature on enzyme activity, enzyme inhibition.

Unit II: Biochemistry of Disease: A diagnostic approach by blood/ urine analysis

Blood: Composition and functions of blood, blood coagulation. Blood collection and preservation of samples. Anaemia, Regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin.

Urine: Collection and preservation of samples. Formation of urine. Composition and estimation of constituents of normal and pathological urine.

Unit III: Practical

Identification and estimation of the following:
[1] Carbohydrates – qualitative and quantitative.
[2] Lipids – qualitative.
[3] Determination of the iodine number of oil.
[4] Determination of the saponification number of oil.
[5] Determination of cholesterol using Liebermann- Burchard reaction.
[6] Proteins – qualitative.
[7] Isolation of protein.
[8] Determination of protein by the Biuret reaction.
[9] Determination of nucleic acids

Suggested Readings:

[1] T.G. Cooper: *Tool of Biochemistry*;
[2] G. P. Talwar and M Srivastava: *Textbook of Biochemistry and Human Biology*.
[3] A.L. Lehninger: *Biochemistry*.
[2] Keith Wilson and John Walker: *Practical Biochemistry*.
[3] Alan H Gowenlock: *Varley's Practical Clinical Biochemistry*.

Skill Enhancement Course

CYS-111: Green Methods in Chemistry

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 01 + Practical: 01)
Total Hours	:	15 Theory + 30 Practical
Lectures	:	01 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand green chemistry, and its need, goals, limitations and principles
[CO.2] To know and understand alternate routes for the green synthesis of some organic compounds
[CO.3] To know and understand the use of microwaves as the source of energy for carrying out the reactions in water
[CO.4] To know and understand the use of ultra sound for performing reactions in water
[CO.5] To know and understand the future trends in green chemistry

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will understand green chemistry, and its need, goals, limitations and principles
[CO.2] Student(s) will know and understand alternate routes for the green synthesis of some organic compounds
[CO.3] Student(s) will know and understand the use of microwaves as the source of energy for carrying out the reactions in water
[CO.4] Student(s) will know and understand the use of ultra sound for performing reactions in water
[CO.5] Student(s) will know and understand the future trends in green chemistry

COURSE CONTENT

Tools of Green chemistry, Twelve principles of Green Chemistry, with examples.

The following Real-world Cases in Green Chemistry should be discussed:
[1] A green synthesis of ibuprofen which creates less waste and fewer byproducts (Atom economy).
[2] Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO_2 for precision cleaning and dry cleaning of garments.
[3] Environmentally safe antifoulant.
[4] CO_2 as an environmentally friendly blowing agent for the polystyrene foam sheet packaging market.
[5] Using a catalyst to improve the delignifying (bleaching) activity of hydrogen peroxide.
[6] A new generation of environmentally advanced preservative: getting the chromium and arsenic out of pressure treated wood.
[7] Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
[8] Development of a fully recyclable carpet: cradle to cradle carpeting.

Suggested Readings

[1] Manahan S.E. (2005) *Environmental Chemistry*, CRC Press
[2] Miller, G.T. (2006) *Environmental Science* 11th edition. Brooks/Cole
[3] Mishra, A. (2005) *Environmental Studies*. Selective and Scientific Books, New

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Skill Enhancement Course

CYS-112: Pharmaceutical Chemistry

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	02 (Theory: 01 + Practical: 01)
Total Hours	:	15 Theory + 30 Practical
Lectures	:	01 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand drug discovery, design and development.
[CO.2] To learn how to synthesize the representative drugs of the important classes including analgesics agents, antipyretic agents, anti-inflammatory agents, antibiotics, antibacterial and antifungal agents, antiviral agents, central nervous system agents, cardiovascular, antilaprosy and HIV-AIDS related drugs.
[CO.3] To know and understand the difference between aerobic and anaerobic fermentation.
[CO.4] To know the chemical routes involved in the production of (i) ethyl alcohol and citric acid, (ii) penicillin, cephalosporin, chloromycetin and streptomycin, (iii) lysine, glutamic acid, vitamin B2, vitamin B12 and Vitamin C.
[CO.5] To learn how to prepare and synthesize aspirin in laboratory and analyse it
[CO.6] To learn how to prepare and synthesize magnesium bisilicate (antacid) in the laboratory

Course Outcomes:

After completion of this course,
[CO.1] Student(s) will know and understand drug discovery, design and development.
[CO.2] Student(s) will have the skills to synthesize the representative drugs of the important classes including analgesics agents, antipyretic agents, anti-inflammatory agents, antibiotics, antibacterial and antifungal agents, antiviral agents, central nervous system agents, cardiovascular, antilaprosy and HIV-AIDS related drugs.
[CO.3] Student(s) will know and understand the difference between aerobic and anaerobic fermentation.
[CO.4] Student(s) will know about the chemical routes involved in the production of (i) ethyl alcohol and citric acid, (ii) penicillin, cephalosporin, chloromycetin and streptomycin, (iii) lysine, glutamic acid, vitamin B2, vitamin B12 and Vitamin C.
[CO.5] Student(s) will have the skills to prepare and synthesize aspirin in laboratory and analyse it
[CO.6] Student(s) will have the skills to prepare and synthesize magnesium bisilicate (antacid) in the laboratory

COURSE CONTENT

Unit I: Pharmaceutical Compounds: Structure and Importance

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis). An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

Unit II: Drugs

Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol, lbuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

Unit III: Fermentation

Aerobic and anaerobic fermentation. Production of (i) Ethyl alcohol and citric acid, (ii) Antibiotics; Penicillin, Cephalosporin, Chloromycetin and Streptomycin, (iii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C.

Unit IV: Practicals

[1] To prepare aspirin and carry out its analysis.
[2] To prepare magnesium bisilicate (Antacid).
[3] To understand chemistry and production of amoxicillin.

Suggested Readings

[1] G.L. Patrick: *Introduction to Medicinal Chemistry*, Oxford University Press, UK.
[2] Hakishan, V.K. Kapoor: *Medicinal and Pharmaceutical Chemistry*, Vallabh Prakashan, New Delhi.
[3] William O. Foye, Thomas L., Lemke, David A. William: *Principles of Medicinal Chemistry*, B.I. Waverly Pvt. Ltd. New Delhi.
[4] Lab Manual, Li, Roy & Fortenberry, University of Mississippi, USA
[5] P.S. Kalsi, "*Spectroscopy of Organic Compounds*" 9th Edition (2022), New Age Publishers.
[6] Jiben Roy, "*A Self-Study Guide to the Principles of Organic Chemistry*" Universal Publishers.
[7] P.S. Kalsi, "*Pharmaceutical Organic Chemistry*" (2022 Edition).

Discipline Specific Elective (DSE) Courses: (Credit: 04 each)

1. Polymer Chemistry (04 Credits)
2. Inorganic Materials for Industrial Applications (04 Credits)
3. Novel Inorganic Solids (04 Credits)
4. Research Methodology for Chemistry (05 Credits)
5. Applications of Computers in Chemistry (04 Credits)
6. Molecular Modelling & Drug Design (04 Credits)
7. Industrial Chemicals & Environment (04 Credits)
8. Minor Dissertation

Note: Universities may include more options or delete some from this list

Discipline Specific Elective Course: 04 Credits

CYE-101: Polymer Chemistry

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the history, classification and nomenclature of polymers, molecular forces and chemical bonding in polymers, texture of polymers, criteria for synthetic polymer formation, classification of polymerization processes, and relationships between functionality

[CO.2] To know and understand the mechanism and kinetics of step growth, radical chain growth, ionic chain and coordination polymerizations, the mechanism and kinetics of copolymerization and polymerization techniques.

[CO.3] To know and understand the crystallization and crystallinity of polymers

[CO.4] To know and understand the structure property relationships in polymers

[CO.5] To understand the molecular weight(s) and glass transition temperature of polymers, physical, thermal, flow & mechanical properties of polymers

[CO.6] To learn how to carry out various polymerization reactions such as free radical solution polymerization, redox polymerization, and precipitation polymerization, and microscale emulsion polymerization

[CO.7] To learn how to prepare and synthesize simple polymers such as nylon 66/6, polyester, urea-formaldehyde resin, novalac resin/resold resin and poly(methylacrylate).

[CO.8] To learn how to characterize the polymers by determining the molecular weight using different methods such as viscometry, and end group analysis.

Course Outcomes:

After completion of this course,

[CO.1] Student(s) will know and understand the polymers, molecular forces and chemical bonding in polymers, texture of polymers, criteria for synthetic polymer formation, classification of polymerization processes, and relationships between functionality.

[CO.2] Student(s) will know and understand the mechanism and kinetics of step growth, radical chain growth, ionic chain and coordination polymerizations, the mechanism and kinetics of copolymerization and polymerization techniques.

[CO.3] Student(s) will understand the crystallization and crystallinity of polymers, the structure property relationships in polymers, molecular weight(s) and glass transition temperature of polymers.

[CO.4] Student(s) will understand physical, thermal, flow & mechanical properties of polymers.

[CO.5] Student(s) will have the skills to carry out various polymerization reactions such as free radical solution polymerization, redox polymerization, and precipitation polymerization, and microscale emulsion polymerization.

[CO.6] Student(s) will have the skills to prepare and synthesize simple polymers such as nylon 66/6, polyester, urea-formaldehyde resin, novalac resin/resold resin and poly(methylacrylate).

[CO.7] Student(s) will have the skills to characterize the polymers by determining the molecular weight using different methods such as viscometry, and end group analysis.

COURSE CONTENT

Unit I: Introduction and History of Polymeric Materials

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers.

Unit II: Functionality and its Importance

Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bifunctional systems, Poly-functional systems.

Unit III: Kinetics of Polymerization

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

Unit IV: Crystallization and Crystallinity

Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point. Glass Transition Temperature (Tg), Factors affecting glass transition temperature (Tg). Structure Property relationships

Unit V: Determination of Molecular Weight of Polymers (***Mn***, ***Mw***, etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance.

Polydispersity index.

Unit VI: Polymer Solution:

Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures.

Unit VII: Laboratory Experiments

[A] On Polymer Synthesis

[1] To prepare nylon 66/6
[2] To carry out redox polymerization of acrylamide
[3] To carry out precipitation polymerization of acrylonitrile
[4] To carry out the preparation of urea-formaldehyde resin
[5] To prepare novalac resin/resold resin.
[6] To carry out the microscale Emulsion Polymerization of Poly(methylacrylate).

[B] Polymer Characterization

[1] To use viscometry for determination of molecular weight of *Polyacrylamide-aq. $NaNO_2$ solution,*
[2] To use viscometry for determination of molecular weight of *Poly vinyl proplylidine (PVP) in water*
[3] To determine the viscosity-average molecular weight of poly(vinyl alcohol) i.e., PVOH and the fraction of "head-to-head" monomer linkages in the polymer.

Suggested Readings

[1] Seymour's *Polymer Chemistry*, Marcel Dekker, Inc.
[2] G. Odian: *Principles of Polymerization*, John Wiley.
[3] F.W. Billmeyer: *Text Book of Polymer Science*, John Wiley.
[4] P. Ghosh: *Polymer Science & Technology*, Tata Mcgraw-Hill.
[5] R.W. Lenz: *Organic Chemistry of Synthetic High Polymers*.
[6] Malcohm P. Stevens, *Polymer Chemistry: An Introduction*, 3rd Ed.
[7] Harry R. Allcock, Frederick W. Lampe and James E. Mark, *Contemporary Polymer Chemistry*, 3rd ed. Prentice-Hall (2003).

Discipline Specific Elective Course: 04 Credits

CYE-102: Inorganic Materials for Industrial Applications

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand (i) inorganic materials (such as glass, ceramics and cements) of silicate industries, (ii) the types and manufacturing of common fertilizers, (iii) surface coating, its classification, paints and pigments, fillers, thinners, enamels, and emulsifying agents.
[CO.2] To know and understand the dyes, wax polishing, water and oil paints, additives, metallic coatings (electrolytic and electroless), metal spraying and anodizing, batteries, their components and working of different types of batteries, alloys and their classification, types of alloys, specific properties of elements in alloys, and manufacturing of steel
[CO.3] To learn how to analyse the inorganic materials or compounds (such as fertilizers, cement, alloys, pigments) of industrial importance
[CO.4] To learn how to determine (i) free acidity in ammonium sulphate fertilizer, (ii) composition of dolomite with the help of complexometric titration.
[CO.5] To learn how to estimate (i) calcium in calcium ammonium nitrate fertilizer, (ii) phosphoric acid in superphosphate fertilizer, (iii)
[CO.6] To learn how to analyse cement and alloys or synthetic samples.
[CO.7] To learn how to prepare the pigment (zinc oxide).

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will know and understand (i) inorganic materials (such as glass, ceramics and cements) of silicate industries, (ii) the types and manufacturing of common fertilizers, (iii) surface coating, its classification, paints and pigments, fillers, thinners, enamels, and emulsifying agents.
[CO.2] Student(s) will know and understand the dyes, wax polishing, water and oil paints, additives, metallic coatings (electrolytic and electroless), metal spraying and anodizing, batteries, their components and working of different types of batteries, alloys and their classification, types of alloys, specific properties of elements in alloys, and manufacturing of steel
[CO.3] Student(s) will have the skills to analyse the inorganic materials or compounds (such as fertilizers, cement, alloys, pigments) of industrial importance
[CO.4] Student(s) will have the skills to determine (i) free acidity in ammonium sulphate fertilizer, (ii) composition of dolomite with the help of complexometric titration.
[CO.5] Student(s) will have the skills to estimate (i) calcium in calcium ammonium nitrate fertilizer, (ii) phosphoric acid in superphosphate fertilizer, (iii)
[CO.6] Student(s) will have the skills to analyse cement and alloys or synthetic samples.
[CO.7] Student(s) will have the skills to prepare the pigment (zinc oxide).

COURSE CONTENT

Unit I: Silicate Industries

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

Unit II: Fertilizers

Different types of fertilizers. Manufacture of the fertilizers including urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

Unit III: Surface Coatings

Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

Unit IV: Batteries

Primary and secondary batteries, battery components and their role, Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell.

Unit V: Alloys

Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

Unit VI: Laboratory Experiments

[1]. To determine free acidity in ammonium sulphate fertilizer.
[2]. To estimate Calcium in Calcium ammonium nitrate fertilizer.
[3]. To estimate the phosphoric acid in superphosphate fertilizer.
[4]. To perform electroless metallic coatings on ceramic and plastic material.
[5]. To determine the composition of dolomite (by complexometric titration).
[6]. To analyse (Cu, Ni); (Cu, Zn) in alloy or synthetic samples.
[7]. To carry out the analysis of Cement.
[8]. To prepare the pigment (zinc oxide).

Suggested Readings

[1] B. K. Sharma: *Engineering Chemistry*, Goel Publishing House, Meerut.
[2] E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
[3] R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
[4] W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
[5] J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
[6] P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
[7] R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi

Discipline Specific Elective Course: 04 Credits

CYE-103: Novel Inorganic Solids

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the methods of synthesis and modification of inorganic solids
[CO.2] To know and understand the inorganic solids (solid electrolytes, mixed inorganic pigments, molecular material) of technological importance
[CO.3] To know and understand the nanomaterials and their classification, Au and Ag nanostructures, carbon nanotubes and inorganic nanowires.
[CO.4] To know and understand the composition, mechanical and fabricating characteristics and applications of various types of engineering materials (e.g., cast irons, plain carbon and alloy steels).
[CO.5] To know and understand composite materials, environmental effects on composites and applications
[CO.6] To know and understand ion exchange resins and their applications, ceramic and refractory materials and their applications.
[CO.7] To learn how to use the methods for the determination of novel inorganic solids.
[CO.8] To learn how to apply cation exchange method
[CO.3] To learn how to determine total difference of solids.
[CO.4] To learn how to synthesize (i) hydrogel by co-precipitation method (ii) silver and gold metal nanoparticles.

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will understand the methods of synthesis and modification of inorganic solids.
[CO.2] Student(s) will know and understand the inorganic solids (solid electrolytes, mixed inorganic pigments, molecular material) of technological importance.
[CO.3] Student(s) will know and understand the nanomaterials and their classification, Au and Ag nanostructures, carbon nanotubes and inorganic nanowires.
[CO.4] Student(s) will know and understand the composition, mechanical and fabricating characteristics and applications of various types of engineering materials (e.g., cast irons, plain carbon and alloy steels).
[CO.5] Student(s) will know and understand composite materials, environmental effects on composites and applications.
[CO.6] Student(s) will know and understand ion exchange resins and their applications, ceramic and refractory materials and their applications.
[CO.7] Student(s) will have the skills to use the methods for determining novel inorganic solids.
[CO.8] Student(s) will have the skills to apply cation exchange method.
[CO.9] Student(s) will have the skills to determine total difference of solids.
[CO.10] Student(s) will have the skills to synthesize (i) hydrogel by co-precipitation method (ii) silver and gold metal nanoparticles.

COURSE CONTENT

Unit I: Synthesis and Modification of Inorganic Solids

Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods.

Unit II: Inorganic Solids of Technological Importance

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments.

Unit III: Nanomaterials

Overview of nanostructures and nanomaterials: classification.

Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires.

Unit IV: Introduction to Engineering Materials for Mechanical Construction

Composition, mechanical and fabricating characteristics and applications of various types of cast irons, plain carbon and alloy steels.

Unit V: Composite Materials

Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, environmental effects on composites, applications of composites.

Unit VI: Speciality Polymers

Ion-exchange resins and their applications. Ceramic & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications.

Unit VI: Laboratory Experiments

[1] Determination of cation exchange method
[2] Determination of total difference of solids.
[3] Synthesis of hydrogel by co-precipitation method.
[4] Synthesis of silver and gold metal nanoparticles.

Suggested Readings

[1] *Seymour's Polymer Chemistry*, Marcel Dekker, Inc.
[2] G. Odian: *Principles of Polymerization*, John Wiley.
[3] F.W. Billmeyer: *Text Book of Polymer Science*, John Wiley.
[4] P. Ghosh: *Polymer Science & Technology*, Tata Mcgraw-Hill.
[5] R.W. Lenz: *Organic Chemistry of Synthetic High Polymers*.
[6] Fahan, *Materials Chemistry*, Springer (2004).

Discipline Specific Elective Course: 06 Credits

CYE-104: Research Methodology for Chemistry

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Tutorial: 01)
Total Hours	:	45 Theory + 15 Tutorial
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

Course Objectives:

[CO.1] To know and understand the printed sources of information for literature survey, digital sources of information for literature survey, and information technology and library resources

[CO.2] To know and understand the methods of scientific research and writing scientific papers, writing ethics, and avoiding plagiarism.

[CO.3] To know and understand the chemical safety and ethical handling of chemicals, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards.

[CO.4] To know and understand the data analysis, the investigative approach, and analysis and presentation of data

Course Outcomes:

After completion of the course,

[CO.1] Students will know and understand the printed sources of information for literature survey, digital sources of information for literature survey, and information technology and library resources.

[CO.2] Students will know and understand the methods of scientific research and writing scientific papers, writing ethics, and avoiding plagiarism.

[CO.3] Students will know and understand the chemical safety and ethical handling of chemicals, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards.

[CO.4] Students will know and understand the data analysis, the investigative approach, and analysis and presentation of data.

COURSE CONTENT

Unit I: Literature Survey

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus.

Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information.

Unit II: Methods of Scientific Research and Writing Scientific Papers

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation.

Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism.

Unit III: Chemical Safety and Ethical Handling of Chemicals

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

Unit IV: Data Analysis

The Investigative Approach: Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments.

Suggested Readings

[1] Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) *Practical skills in chemistry*. 2nd Ed. Prentice-Hall, Harlow.
[2] Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
[3] *How to use Excel in analytical chemistry and in general scientific data analysis*. Cambridge Univ. Press (2001) 487 pages.
[4] *Chemical safety matters – IUPAC – IPCS*, Cambridge University Press, 1992. • OSU safety manual 1.01

Discipline Specific Elective Course: 04 Credits

CYE-105: Applications of Computers in Chemistry

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Tutorial: 01)
Total Hours	:	45 Theory + 15 Tutorial
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

Course Objectives:

[CO.1] To know and understand the basics of computer applications such as constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions.
[CO.2] To know and understand the elements of the basic language, basic keywords and commands, logical and relative operators, strings and graphics.
[CO.3] To know and understand the compiled versus interpreted languages, debugging, simple programs, matrix addition, multiplication, statistical analysis, numerical methods including roots of equations, differential calculus, integral calculus, simultaneous equations, interpolation, extrapolation and curve fitting,
[CO.4] To know and understand the conceptual background of molecular modelling
[CO.5] To learn how to use computer programs (based on numerical methods) for roots of equations (e.g., volume of van der Waals gas and comparison with ideal gas, pH of a weak acid), numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations), numerical integration (e.g., entropy/ enthalpy changes from heat capacity data), probability distributions (gas kinetic theory) and mean values.
[CO.6] To learn how to use computer programs (based on numerical methods) for Matrix operations and their application of Gauss-Siedel method in colourimetry.
[CO.7] To learn how to use molecular visualization software, and carry out simple exercise.

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will understand basics of computer applications such as constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions.
[CO.2] The student(s) will know and understand the elements of the basic language, basic keywords and commands, logical and relative operators, strings and graphics.
[CO.3] The student(s) will know and understand the compiled versus interpreted languages, debugging, simple programs, matrix addition, multiplication, statistical analysis, numerical methods including roots of equations, differential calculus, integral calculus, simultaneous equations, interpolation, extrapolation and curve fitting,
[CO.4] The student(s) will know and understand the conceptual background of molecular modelling
[CO.5] Student(s) will have the skills to use computer programs (based on numerical methods) for roots of equations (e.g., volume of van der Waals gas and comparison with ideal gas, pH of a weak acid), numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations), numerical integration (e.g. entropy/ enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values.
[CO.6] The student(s) will have the skills to use computer programs (based on numerical methods) for Matrix operations and their application of Gauss-Siedel method in colourimetry.
[CO.7] The student(s) will have the skills to use molecular visualization software, and carry out simple exercises.

COURSE CONTENT

Unit I: Basics

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands.

Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

Unit II: Numerical Methods

Roots of equations: Numerical methods for roots of equations: Quadratic formula, iterative method, Newton-Raphson method, Binary bisection and Regula-Falsi.

Differential calculus: Numerical differentiation.

Integral calculus: Numerical integration (Trapezoidal and Simpson's rule), probability distributions and mean values.

Simultaneous equations: Matrix manipulation: addition, multiplication. Gauss-Siedal method.

Interpolation, extrapolation and curve fitting: Handling of experimental data.

Conceptual background of molecular modelling: Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

Unit III: Laboratory

Computer programs based on numerical methods for

[1] Roots of equations: (e.g., volume of van der Waals gas and comparison with ideal gas, pH of a weak acid).
[2] Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
[3] Numerical integration (e.g., entropy/ enthalpy changes from heat capacity data), probability distributions (gas kinetic theory) and mean values.
[4] Matrix operations. Application of Gauss-Siedel method in colourimetry.
[5] Simple exercises using molecular visualization software.

Suggested Readings

[1] Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
[2] Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
[3] Noggle, J. H. *Physical chemistry on a Microcomputer*. Little Brown & Co. (1985).
[4] Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).
[5] McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
[6] Mortimer, R. *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier (2005).
[7] Steiner, E. *The Chemical Maths Book*, Oxford University Press (1996).
[8] Yates, P. *Chemical Calculations*. 2nd Ed. CRC Press (2007).
[9] Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
[10] Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.

Discipline Specific Elective Course: 04 Credits

CYE-106: Molecular Modelling and Drug Design

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Tutorial: 01)
Total Hours	:	45 Theory + 15 Tutorial
Lectures	:	03 per week
Tutorial	:	01 per week
Practical	:	0

Course Objectives:

[CO.1] To know and understand the concepts of molecular modelling, computer hardware and software, and the molecular modelling literature.
[CO.2] To know and understand the force fields including bond stretching, angle bending, non-bonded interactions, electrostatic interactions, van der Waals Interactions and H-bonding
[CO.3] To know and understand energy minimization, computer simulation, molecular dynamics, Monte Carlo simulation.
[CO.4] To know and understand structure prediction and drug design, predicting protein structures by 'Threading', molecular docking, drug discovery – chemoinformatics – QSAR.
[CO.5] To learn how to use various softwares including ChemSketch, ArgusLab (www.planaria-software.com), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer, Hyperchem.
[CO.6] To learn how to compare the optimized C-C bond lengths and visualize the molecular orbitals.
[CO.7] To learn how to carry out conformational analysis of simple unsaturated organic molecules and determine the enthalpy of isomerization of *cis* and *trans-isomers* of such compounds.
[CO.8] To learn how to compare the shapes of the simple organic molecules, and show how the shapes affect the boiling points.
[CO.9] To learn how to visualize the electron density and electrostatic potential maps for diatomic inorganic compounds.
[CO.10] To learn how to build and minimize organic compounds
[CO.11] To learn how to determine the heat of hydration of ethylene, and compute the resonance energy of benzene

Course Objectives:

After completion of the course,
[CO.1] Student(s) will know and understand the concepts of molecular modelling, computer hardware and software, the molecular modelling literature, force fields (including bond stretching, angle bending, non-bonded interactions, electrostatic interactions, van der Waals Interactions and H-bonding), energy minimization, computer simulation, molecular dynamics, Monte Carlo simulation, structure prediction and drug design, predicting protein structures by 'Threading', molecular docking, drug discovery – chemoinformatics – QSAR.
[CO.2] Student(s) will have the skills to use various softwares including ChemSketch, ArgusLab (www.planaria-software.com), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer, Hyperchem.
[CO.3] Student(s) will have the skills to compare the optimized C−C bond lengths and visualize the molecular orbitals.
[CO.4] Student(s) will have the skills to carry out conformational analysis of simple organic molecules and determine the enthalpy of isomerization of *cis* and *trans-isomers* of such compounds.
[CO.5] Student(s) will have the skills to compare the shapes of the simple organic molecules, and show how the shapes affect the boiling points.
[CO.6] Student(s) will have the skills to visualize the electron density and electrostatic potential maps for diatomic inorganic compounds.
[CO.7] Student(s) will have the skills to build and minimize organic compounds.
[CO.8] Student(s) will have the skills to determine the heat of hydration of ethylene, and compute the resonance energy of benzene.

COURSE CONTENT

Unit I: Introduction to Molecular Modelling

Introduction. Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature.

Unit II: Force Fields

Fields. Bond Stretching. Angle Bending. Introduction to nonbonded interactions. Electrostatic interactions. van der Waals Interactions. Hydrogen bonding in Molecular Mechanics. Force Field Models for the Simulation of Liquid Water.

Unit III: Energy Minimization and Computer Simulation

Minimization and related methods for exploring the energy surface. Non-derivative method, First and second order minimization methods. Computer simulation methods. Simple thermodynamic properties and Phase Space. Boundaries. Analyzing the results of a simulation and estimating Errors.

Unit IV: Molecular Dynamics & Monte Carlo Simulation

Molecular Dynamics Simulation Methods. Molecular Dynamics using simple models. Molecular Dynamics with continuous potentials. Molecular Dynamics at constant temperature and pressure. Metropolis method. Monte Carlo simulation of molecules. Models used in Monte Carlo simulations of polymers.

Unit V: Structure Prediction and Drug Design

Structure prediction - Introduction to comparative Modeling. Sequence alignment. Constructing and evaluating a comparative model. Predicting protein structures by 'Threading', Molecular docking. Structure based de novo ligand design,

Drug Discovery – Chemoinformatics – QSAR.

Unit VI: Laboratory Experiments

[1] To compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.

[2] (a) To perform a conformational analysis of butane. (b) To determine the enthalpy of isomerization of *cis* and *trans* 2-butene.

[3] To visualize the electron density and electrostatic potential maps for LiH, HF, N2, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.

[4] (a) To relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) To compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.

[5] (a) To compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) To show how the shapes affect the trend in boiling points: (118 ºC, 100 ºC, 108 ºC, 82 ºC, respectively).

[6] To build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) *alkyl halide* (b) *aldehyde* (c) *ketone* (d) *amine* (e) *ether* (f) *nitrile* (g) *thiol* (h) *carboxylic acid* (i) *ester* (j) *amide*.

[7] (a) To determine the heat of hydration of ethylene. (b) To compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.

[8] To arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.

[9] (a) To compare the optimized bond angles H_2O, H_2S, H_2Se. (b) To compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.

Note: Software: ChemSketch, ArgusLab (www.planaria-software.com), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer, Hyperchem, or any similar software.

Suggested Readings

[1] A.R. Leach, *Molecular Modelling Principles and Application*, Longman, 2001.
[2] J.M. Haile, *Molecular Dynamics Simulation Elementary Methods*, John Wiley and Sons, 1997.
[3] Satya Prakash Gupta, *QSAR and Molecular Modeling*, Springer - Anamaya Publishers, 2008
[4] A.R. Leach, *Molecular Modelling Principles and Application*, Longman, 2001.
[5] J.M. Haile, *Molecular Dynamics Simulation Elementary Methods*, John Wiley and Sons, 1997.
[6] Satya Prakash Gupta, *QSAR and Molecular Modeling*, Springer - Anamaya Publishers, 2008.

Discipline Specific Elective Course: 04 Credits

CYE-107: Industrial Chemicals & Environment

(Non-Semester Specific)

Type	:	Elective Course
Total Credits	:	04 (Theory: 03 + Practical: 01)
Total Hours	:	45 Theory + 30 Practical
Lectures	:	03 per week
Tutorial	:	0
Practical	:	01 per week

Course Objectives:

[CO.1] To know and understand the industrial gases, inorganic chemicals, the preparation of metals / ultrapure metals for semiconductor technology, the impact of air pollutants on environment, impact of water pollutants on environment, water purification methods, industrial waste management, sources of energy (e.g., coal, petrol, natural gas, and nuclear fuels) and related aspects of pollution

[CO.2] To know and understand biocatalysis and its importance in green chemistry and chemical industry

[CO.3] To learn how to analyse water or aqueous samples and determine (i) dissolved oxygen, (ii) dissolved CO_2, (ii) chemical oxygen demand (COD), biological oxygen demand (BOD), (iii) content of chloride, sulphate, carbonate (CO_3^{2-}) and bicarbonate (HCO_3^-) ions, (iv) salinity and total alkalinity of such water samples.

[CO.4] To learn how to estimate SPM in air samples

[CO.5] To learn how to determine percentage of available chlorine in bleaching powder.

[CO.5] To learn about the common bio-indicators of pollution.

[CO.6] To learn how to prepare and synthesize borax/ boric acid.

Course Outcomes:

After completion of the course,

[CO.1] Student(s) will know and understand the industrial gases, inorganic chemicals, the preparation of metals / ultrapure metals for semiconductor technology, the impact of air pollutants on environment, impact of water pollutants on environment, water purification methods, industrial waste management, sources of energy (e.g., coal, petrol, natural gas, and nuclear fuels) and related aspects of pollution

[CO.2] Student(s) will understand importance of biocatalysis in green chemistry and industry.

[CO.3] Student(s) will have the skills to analyse water or aqueous samples and determine (i) dissolved oxygen, (ii) dissolved CO_2, (ii) chemical oxygen demand (COD), biological oxygen demand (BOD), (iii) content of chloride, sulphate, carbonate (CO_3^{2-}) and bicarbonate (HCO_3^-) ions, (iv) salinity and total alkalinity of such water samples.

[CO.4] Student(s) will have the skills to estimate SPM in air samples

[CO.5] Student(s) will have the skills to (i) determine percentage of available chlorine in bleaching powder, and (ii) to understand and interpret the common bio-indicators of pollution.

[CO.6] Student(s) will have the skills to prepare and synthesize borax/ boric acid.

Course Content

Unit I: Industrial Gases and Inorganic Chemicals

Industrial Gases: Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene.

Inorganic Chemicals: Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.

Unit II: Industrial Metallurgy

Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconduct or technology.

Unit III: Environment and its Segments

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

Air Pollution: Major regions of atmosphere. Chemical and photochemical reactions in atmosphere.

Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Environmental effects of ozone, Major sources of air pollution.

Pollution by SO_2, CO_2, CO, NO*x*, H_2S and other foul-smelling gases. Methods of estimation

of CO, NO*x*, SO*x* and control procedures.

Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates.

Water Pollution: Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems.

Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment).

Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. Sludge disposal.

Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

Unit IV: Energy & Environment

Sources of Energy: Coal, petrol and natural gas. Nuclear Fusion / Fission, Solar energy, Hydrogen, geothermal, Tidal and Hydel, etc.

Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management.

Unit V: Biocatalysis

Introduction to biocatalysis: Importance in "Green Chemistry" and Chemical Industry.

Unit VI: Laboratory Experiments

[1] To determine the dissolved oxygen in water.
[2] To determine the Chemical Oxygen Demand (COD).
[3] To determine the Biological Oxygen Demand (BOD).
[4] To determine the percentage of available chlorine in bleaching powder.
[5] To measure the chloride, sulphate and salinity of water samples by simple titration method ($AgNO_3$ and potassium chromate).
[6] To estimation the total alkalinity (CO_3^{2-}, HCO_3^-) of water samples using double titration method.
[7] To measure the dissolved CO_2.
[8] To study some of the common bio-indicators of pollution.
[9] To estimate SPM in air samples.
[10] To prepare borax/ boric acid.

Suggested Readings

[1] E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
[2] R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
[3] J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
[4] S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
[5] K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
[6] S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.
[7] S.E. Manahan, *Environmental Chemistry*, CRC Press (2005).
[8] G.T. Miller, *Environmental Science*, 11th edition. Brooks/ Cole (2006).
[9] A. Mishra, *Environmental Studies*. Selective and Scientific Books, New Delhi (2005).

Discipline Specific Elective Course

CYE-401: Synthetic Organic Chemistry Lab

(For the students at 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 0 + Practical: 4)
Total Hours	:	0 Theory + 120 Practicals
Lectures	:	0
Tutorial	:	0
Practical	:	04 per week

Course Objectives:

[CO.1] To learn how to carry out organic reactions such as bromination reaction, nitration, reaction, Cannizaro reaction, aldol condensation, oxidation reaction, Sandmeyer reaction, Knoevenagel condensation, Wittig reaction, Diels Alder reaction, Friedel Crafts reaction, Fisher indole synthesis etc

[CO.2] To learn how to synthesize and purify the organic compounds.

Course Outcomes:

After completion of the course,

[CO.1] Student(s) will have the skills to carry out organic reactions such as bromination reaction, nitration, reaction, Cannizaro reaction, aldol condensation, oxidation reaction, Sandmeyer reaction, Knoevenagel condensation, Wittig reaction, Diels Alder reaction, Friedel Crafts reaction, Fisher indole synthesis etc

[CO.2] Student(s) will have the skills to synthesize and purify the organic compounds.

COURSE CONTENT

[1] Separation of organic mixtures by TLC and PTLC.

[2] Synthesis of derivatives for carbonyl, amino and active methylene compounds.

[3] Nitration of methyl benzoate

[4] Bromination of acetanilide.

[5] Preparation of *p*-nitroaniline of acetanilide

[6] Cannizzaro reaction of an aromatic Aldehyde (*p*-nitrobenzaldehyde).

[7] Aldol condensation (benzaldehyde + acetone or cinnamaldehyde + acetone)

[8] Oxidation of hydroquinone to p-benzoquinone.

[9] Oxidation of benzoin to benzyl.

[10] Conversion of benzyl to quinoxaline.

[11] Reduction of Camphor.

[12] Synthesis of 2-iodobenzoic acid by Sandmeyer reaction.

[13] Synthesis of binapthol by green reaction.

[14] Knoevenagel condensation between aldehyde (4-diethylaminobenzaldehyde) and malonic acid, cyanoacetic acid or malononitrile.

[15] Friedel-Crafts reaction: synthesis of l ,*4-di-tert-butyl-2,5*-dimethoxy benzene.

[16] Diels-Alder reaction between anthracene and maleic anhydride.

[17] Preparation and purification of *cis*- and trans-stilbenes by Wittig reaction.

[18] Preparation of pyridium dichromate and its uses in oxidation of benzyl alcohol.

[19] Synthesis of ω-nitrostyrene from an aromatic aldehyde and nitromethane

[20] Synthesis of chalcone from an aromatic aldehyde and acetophenone.

[21] Extraction of oils from ground nuts using Soxhlet apparatus

[22] Synthesis of α-bromo cinnamic acid or phenyl acetylene from benzaldehyde, (formation of cinnamic acid, bromination and elimination reactions).

[23] Preparation of *meso*-stilbene dibromide and its conversion to diphenylacetylene.

[24] Fisher indole synthesis.

Note: Some experiments would require two-three turns, and minimum ten experiments must be done.

Suggested Readings

[1] Arthur, I. V.," *Quantitative Organic Analysis,"* Pearson.
[2] Furniss, B.S., Handford, A. J., Smith P. W. G. & Tatchell A. R., *"Vogel's Text Book of Practical Organic Chemistry"* 5th Ed. Longman (1996).
[3] Leonard J., Lygo B. & Procter G., *"Advanced Practical Organic Chemistry"*, Champan and Hall. (1995)
[4] Mann, F. G. & Saunders, B.C. *"Practical Organic Chemistry"*, Pearson. (2009)
[5] Furniss, B.S., Handford, A. J., Smith P. W. G. & Tatchell A. R., *"Practical Organic Chemistry"* 5th Ed., Pearson.
[6] Arthur, I. V. *Quantitative Organic Analysis*, Pearson.

7th or 8th Semester

CYE-402: Structure and Reactivity of Organic Molecules

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the conformations and reactivities of cyclohexane and its derivatives.
[CO.2] To know and understand various models to predict stereochemical outcomes of nucleophilic additions to carbonyl compounds.
[CO.3] To know and understand the thermodynamics and kinetics aspects of a chemical reactions.
[CO.4] To know and understand various methods for elucidation of reaction mechanism.
[CO.5] To know and understand different types of catalysis in organic reactions.

Course Outcomes:

After completion of the course,
[CO.1] Students will understand the conformations and reactivities of cyclohexane and its derivatives.
[CO.2] Students will know and understand various models to predict stereochemical outcomes of nucleophilic additions to carbonyl compounds.
[CO.3] Students will know the thermodynamics and kinetics aspects of a chemical reactions.
[CO.4] Students will know and understand various methods for elucidation of reaction mechanism.
[CO.5] Students will know and understand different types of catalysis in organic reactions.

COURSE CONTENT

Unit I: Conformational Analysis of Cyclic Systems

Cyclohexane and its derivatives (mono-, di- and tri-substituted), fused (decalins) and bridged bicyclic systems, dynamic stereochemistry, conformational rigidity and mobility, quantitative correlation between conformation and reactivity, effect of conformation on the reduction of cyclic ketones, nucleophilic addition to carbonyl group (Cram, Karabatsos, Felkin-Ahn models, Cieplak effect), nucleophilic substitution on cyclohexane substrates, cyclohexane epoxide formation and opening. elimination reactions of cyclohexyl halides, acetate esters and related compounds, deamination of 2-amino-cyclohexanols, elimination vs substitution competition and neighboring group participation reactions of acyclic and cyclic molecules.

Unit II: Physical Organic Chemistry

Basic concepts, thermodynamic and kinetic requirements, rate and equilibrium constants, reaction coordinate diagram, transition state (activated complex), nature of activated complex, Hammond postulate, reactivity vs selectivity principle, Curtin Hammett principle, microscopic reversibility, kinetic vs thermodynamic control.

Unit III: Methods for Elucidating Mechanism

Kinetic analyses of simple and complex reactions, steady state and saturation kinetics, isotope effects - primary and secondary isotope effects, steric and equilibrium isotope effects, solvent isotope effects, heavy atom isotope effects, substituent effects origin (inductive, field, resonance, steric, solvent and polarizability). Hammett linear free energy relationship, substituent parameter (sigma), reaction constant (rho), use of Hammett plot for mechanism determination, deviation from linearity, inductive vs resonance effects -Taft parameters, nucleophilicity and nucleofugality, factors affecting

nucleophilicity (basicity/acidity, solvation, polarizability and shape), Swain-Scott parameters, Edwards and Ritchie correlations, solvent effects bulk and specific solvent effects, Grunwald-Winstein plots, Bronsted relationships, experiments for identifying mechanism (example Cannizzaro reaction), product and intermediate identification, common intermediate detection (example Ritter reaction and Beckmann fragmentation), trapping and competition experiments, isotope labeling, crossover experiments.

Unit IV: Catalysis

Binding in transition state vs ground state, electrophilic catalysis, acid and base catalysis, nucleophilic, covalent, Bronsted acid base catalysis (general and specific, Bronsted catalysis law, Leffler law), Libido rule.

Suggested Readings

[1] Anslyn, E. V. and Dougherty, D. A., "*Modern Physical Organic Chemistry*", University Science Books.
[2] Clayden, J., Greeves, N. and Warren, S., "*Organic Chemistry*", Oxford University Press.
[3] Carey, F. A. and Sundberg, R. J., "*Advanced Organic Chemistry", Part A: Structure and Mechanisms,* 5th Ed., Springer.
[4] Nasipuri, D., "*Stereochemistry of Organic Compounds: Principles and Applications*" New Age International.
[5] P.S. Kalsi, "*Pharmaceutical Organic Chemistry, 2022 Edition*", New Age International.

7th or 8th Semester

CYE-403: Solid State Chemistry

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the crystal structure and symmetry in the crystalline state

[CO.2] To know and understand the applications of XRD in determine crystal structure and phase of a solid material

[CO.3] To know and understand the hard sphere model, structures derived from HCP and CCP packing, the bonding in solids, band theory, and the properties of solids

Course Outcomes:

After completion of the course,

[CO.1] Students will know and understand the crystal structure and symmetry in the crystalline state.

[CO.2] Students will know and understand the applications of XRD in determine crystal structure and phase of a solid material.

[CO.3] Students will know and understand the hard sphere model, structures derived from HCP and CCP packing, the bonding in solids, band theory, and the properties of solids.

COURSE CONTENT

Unit I: Symmetry in the Crystalline State:

Crystal symmetry, elements of translation-screw axis and glide planes, symmetry in a cube, crystal classes, stereographic projection of crystal systems, space symmetry and space groups, representation of monoclinic and orthorhombic space groups.

Unit II: X-Ray Diffraction:

Crystal planes and directions, Bragg's law in reciprocal space and Ewald sphere, structure factor, integrated intensity and systematic absences/presences, indexing and simulation of powder X-ray diffraction patterns for simple systems.

Unit III: Crystal Chemistry:

Hard sphere model, structures derived from HCP and CCP packing, crystal structures of various compositions, derived structures and polytypes, non-stoichiometry in solids, atomic order/disorder in solids, single crystals, polycrystals, quasicrystals, amorphous / glassy solids.

Unit IV: Bonding in Solids:

Bonding in molecular solids - polymorphism, bonding in extended solids ionic, covalent and metallic. Band theory of solids classification of semiconductors, metals and insulators, free electron theory, Bloch's theorem, concept of density of state and elementary band theory, band structures of one-, two- and three-dimensional solids, selected metals and insulators.

Unit V: Properties of solids:

Thermal, electrical, magnetic and dielectric properties of solids.

Suggested Readings

[1] West, A. R., "*Solid State Chemistry and its Applications*", Reprint, Wiley India.
[2] Rao, C.N.R. and Gopalakrishnan, J., "*New Directions in Solid State Chemistry*", 2nd Ed., Cambridge University Press.
[3] Stout, G.H. and Jensen, L.H., "*X-Ray Structure Determination: A Practical Guide*", 2nd Ed., Wiley-Interscience.
[4] Giacovazzo, C., Artioli, G. and Monaco, H. L., "*Fundamentals of Crystallography*", Oxford University Press.
[5] S. Nicola, "*Magnetic Materials: Fundamentals and Device Applications*", Cambridge University Press.
[6] Cox, P. A., "*The Electronic Structure and Chemistry of Solids*", Oxford University Press.

7th or 8th Semester

CYE-404: Structure and Properties of Metal Complexes

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the stereochemistry and bonding in inorganic compounds of main group elements, metal-ligand bonding, molecular orbital theory, metal-ligand equilibria in solution, electronic spectra of coordination compounds, and

[CO.2] To know and understand the magnetic properties of transition metal complexes

Course Outcomes:

After completion of the course,

[CO.1] Student(s) will know and understand the stereochemistry and bonding in inorganic compounds of main group elements, metal-ligand bonding, molecular orbital theory, metal-ligand equilibria in solution, electronic spectra of coordination compounds, and

[CO.2] Student(s) will know and understand the magnetic properties of transition metal complexes

COURSE CONTENT

Unit I: Stereochemistry and bonding in main group compounds

VSEPR theory, Walsh diagrams (tri- and penta-atomic molecules) dr - pr bonds, bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules, stereoisomerism in inorganic complexes, isomerism arising out of ligand and ligand conformation, chirality and nomenclature of chiral complexes.

Unit II: Metal-ligand bonding and molecular orbital theory (MOT)

Limitations of crystal field theory, d-orbitals splitting in linear, trigonal, octahedral, square planar, tetrahedral and square pyramidal complexes, Jahn-Teller distortion, nephelauxetic series, composition of ligand group orbitals, molecular orbital diagrams of octahedral, tetrahedral, square planar complexes including both σ and π bonding.

Unit III: Metal-ligand equilibria in solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with references to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry an spectrophotometry.

Unit IV: Electronic spectra of coordination compounds

Spectroscopic ground states, correlation and spin-orbit coupling in free ions for 1" series of transition metals, Orgel and Tanabe Sugano diagrams for transition metal complexes (d'- d states), calculation of Dq, B and B parameters, effect of distortion on d-orbital energy levels.

Unit V: Magnetic properties of transition metal complexes

Fundamental equations in molecular magnetism, magnetic susceptibility and magnetic moment, diamagnetic and paramagnetic behaviour of transition metal complexes, spin-orbit coupling effects (L-S coupling and j-j coupling), orbital angular moment and its quenching in octahedral and tetrahedral complexes, temperature independent paramagnetism (TIP) of complexes, spin cross over, ferromagnetic, anti-ferromagnetic, ferrimagnetic behaviour of transition metal compounds, effect of temperature on their magnetic properties.

Suggested Readings

[1] Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M., "*Advanced Inorganic Chemistry*", 6th Ed., John Wiley & Sons, **1999**.

[2] Douglas, B. E., McDaniel, D. H. and Alexander, J. J., "*Concepts and Models in Inorganic Chemistry*", 3rd Ed., John Wiley & Sons, **2001**.

[3] Figgis, B. N., and Hitchman, M. A., "*Ligand Field Theory and Its Applications*", Wiley Eastern Ltd., **1999**.

[4] Huheey, J. E., Keiter, E. A. and Keiter, R. L., "*Inorganic Chemistry Principle of Structure and Reactivity*", 4th Ed, Pearson Education, Inc., **2003**.

[5] Atkins, P., Overton, T., Rourke, J., Mark, W. and Armstrong, F., "*Shriver and Atkins' Inorganic Chemistry*", 4th Ed, Oxford university press, **2009**.

7th or 8th Semester

CYE-405: Methods of Chemical Analysis

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the methods which are used in chemical analysis

[CO.2] To know and understand the principles and instrumentation of electroanalytical methods (such as voltammetry and potentiometry)

[CO.3] To know and understand the principles and instrumentation of thermal methods e.g., TGA, DSC and DTA

Course Outcomes:

After completion of the course,

[CO.1] Student(s) will have the skills to use the methods which are used in chemical analysis

[CO.2] Students will know and understand the principles and instrumentation of electroanalytical methods (such as voltammetry and potentiometry) and thermal methods (e.g., TGA, DSC and DTA)

COURSE CONTENT

Unit I: Introduction:

Brief Introduction of Qualitative Analysis and Quantitative Analysis, Outlines of Various Types of Analytical. Methods of Analysis: Classical Methods and Instrumental Methods. Properties used in various instrumental methods. Basic components of an instrument. Data domains and Types of Analytical Data Domains (Analog Domains, Digital Domains, Time Domains). Selection of An Analytical Mmethod: Precision, Accuracy, Sensitivity, Dynamic Range, Selectivity, Efficiency.

Unit II: Electroanalytical Methods:

Potentiometry & Voltammetry (dependence on technique), Detection of radiation

Unit III: Thermal Methods: TGA, DSC and DTA

Suggested Readings

[1] *Principles of Instrumental Analysis - 6th Edition* by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).

[2] *Instrumental Methods of Analysis, 7th ed*, Willard, Merritt, Dean, Settle.

[3] *P.W. Atkins: Physical Chemistry*.

[4] *G.W. Castellan: Physical Chemistry*.

[5] C.N. Banwell: *Fundamentals of Molecular Spectroscopy*.

[6] Brian Smith*: Infrared Spectral Interpretations: A Systematic Approach*.

[7] W.J. Moore: Physical Chemistry

7th or 8th Semester

CYE-406: Reagents and Reactions in Organic Chemistry

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the reagents which are used in organic reactions and functional group transformations.
[CO.2] To know and understand the methods for C−C, C−N, and C−O single bonds formation.
[CO.3] To know and understand various models for stereochemical aspects of nucleophilic addition to carbonyl compounds.
[CO.3] To know and understand the methods for C−C, C−N, C−O multiple bonds formations.

Course Outcomes:

After completion of the course,
[CO.1] Students will know and understand the reagents which are used in organic reactions and functional group transformations.
[CO.2] Students will know and understand the methods for C−C, C−N, and C−O bonds formation.
[CO.3] Students will know and understand various models for stereochemical aspects of nucleophilic addition to carbonyl compounds.
[CO.3] Students will know and understand methods for C−C, C−N, C−O multiple bonds formations.

COURSE CONTENT

Unit I: Reagents in Organic Synthesis

Use of the following reagents in organic synthesis and functional group transformations; complex metal hydrides organolithium, lithium dimethylcuprate, lithium diisopropylamide (LDA), organomagnesium (Grignard), organozinc, organocopper (Gilman & Normant) reagents in synthesis, dicyclohexylcarbodiimide, 1,3-dithiane (reactivity Umpoloung), trimethylsilyl iodide, tri-*n*-butyltin hydride, Woodward and pervost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, Phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast,

Unit II: Single bond [C—X (X = C, O, N)] formations

Various models (Cram, Cram chelation and Felkin-Anh models) of stereochemical aspects of nucleophilic additions to carbonyls chemistry of enolates (kinetic and thermodynamic) and examines, enolates, lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates, mechanism of aldol (Mukiyama aldol), Stobbe, Darzen, Acyloin condensations, epoxidations (Prilezhaev, Sharpless, Jacobsen and Shi), Metal catalysed C-C bond formations (Ullmann, Buchwald-Hartwig, Sonogashira, Heck, Suzuki, Stille, Nozaki-Hiyama and Kumada reactions).

Unit III: Multiple bond [C—X (X = C, N)] formations

Phosphorus, nitrogen and sulfur ylids, Wittig reaction, Wittig-Honer reaction, Tebbe olefination, Julia olefination, Robinson annulation, Mannich reaction, Peterson olefination, Shapiro reaction, β-eliminations (Hoffman & ester pyrolysis), Cope elimination, selenoxide elimination, Cotey-Winter reaction, olefins from epoxides, olefin metathesis (Schrock's catalyst, Grubb's catalyst, ring closing metathesis, enyne metathesis, Thorpe reaction, Corey-Fuchs reaction, Ohira-Bestmann modification.

Suggested Readings

[1] Carey, F. A. and Sundberg, R.I., "*Advanced organic Chemistry, Part B: Reaction and Synthesis*", 5th Ed. Springer
[2] Anslyn, E. V. and Dougherty, D. A., *"Modern Physical Organic Chemistry",* University Science Books.
[3] Clayden,J, Greeves, N.and Warren, S, *"Organic Chemistry",*Oxford University Press.
[4] Smith, M.B., *"Organic Synthesis",* 3s Ed., Academic Press.
[5] Bruckner, R,, *"Organic Mechanisms: Reactions, Stereochemistry and Synthesis",*Springer.

7th or 8th Semester

CYE-407: Radiation and Photochemistry

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

To know and understand the interaction of high energy radiation with material and induced chemical changes

Course Outcomes:

After completion of the course, the students will know and understand the interaction of high energy radiation with material and induced chemical changes.

COURSE CONTENT

Unit I: Introduction

The scope of radiation chemistry, its relation to other scientific disciplines, the interactions of directly ionising (charged particles) and indirectly ionising (neutrons, photons) radiation with a matter as starting point of radiation-chemical reaction (radiolysis).

Unit II: Primary Intermediate Products (PIP) of Radiolysis, their Formation and Properties:

Excited states, cations, electrons, radicals and anions, Complex excited states: Excimers, exciplexes, plasmons. Superexcited states, Electrons generated by irradiation as the most important agents responsible for the deposition of the radiation energy in a matter, electron degradation spectrum, thermalization and solvation of electrons, Relaxation processes in excited atoms and molecules, Reactions of PIP giving the stable products of radiolysis, Track of an ionising charged particle and its structure, The types of radiation-chemical yields, ionic-pair yield M/N, its meaning and use.

Unit III: Stages of Radiolysis:

Physical stage, physicochemical stage chemical stage and their products. The stage of post-effects (either chemical or biological). The kinetics of radiation-chemical processes.

Unit IV: Radiolysis of Gases and Liquids:

Ionisation in noble gases, the radiolysis of selected gaseous elements, the radiolysis of N_2O and its use in dosimetry, the radiolysis of water vapour, radiolysis of liquid water (including the mechanism, the properties and reactivity of radiolytic products), the influence of conditions during the irradiation on the result of radiolysis, radiolysis of the water solutions of selected inorganic compounds, the radiolysis of solutions containing Fe^{2+} and Ce^{4+} ions, their use in dosimetry.

Unit V: Photochemistry

Quantum efficiencies of photochemical and photophysical processes, experimental techniques for continuous photolysis, Primary and secondary photochemical processes, Franck-Condon principle and its applications, rates of absorption and emission, lifetimes of electronically excited states and their fate, quenching of excited states species-dynamic and static quenching, radiationless transition and pre-dissociation, energy transfer processes.

Suggested Readings

[1] Laidler, K.J., "*Reaction Kinetics*", Anand Sons, New Delhi.

[2] Amis, E.S.,"Solvent Effect of Reaction Rates and Mechanism", Academic Press.

[3] Mukherjee, K.K.,"Fundamentals of Photochemistry", New Age International Pvt. Ltd., New Delhi.

[4] Lakowicz, J.R., "*Principles of Fluorescence Spectroscopy*", Plenum Press, New York.

[5] Wishart, J.F. and Nocera, D.G., "*Photochemistry and Radiation Chemistry*", Oxford University Press, USA.

7th or 8th Semester

CYE-408: Frontiers in Inorganic and Bioinorganic Chemistry

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the reaction mechanisms of transition metal complexes, and electron transfer reactions

[CO.2] To know and understand the photochemistry of metal complexes, and concepts of inorganic biochemistry

[CO.3] To know and understand the chemical toxicity and metallotherapy

Course Outcomes:

After completion of the course,

[CO.1] Student(s) will know and understand the reaction mechanisms of transition metal complexes, and electron transfer reactions

[CO.2] Student(s) will know and understand the photochemistry of metal complexes, and concepts of inorganic biochemistry

[CO.3] Student(s) will know and understand the chemical toxicity and metallotherapy

COURSE CONTENT

Unit I: Reaction Mechanism of Transition Metal Complexes:

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planer complexes, the trans effect.

Unit II: Electron Transfer Reactions

Outer- and inner-sphere mechanisms, factors affecting electron transfer reaction rates, cross reactions and Marcus- Hush theory, solvated electron.

Unit III: Photochemistry of Metal Complexes

Introduction to inorganic photochemistry, photochemically excited states and excited state processes for transition metal complexes, photochemical tractions of coordination compounds, types of photochemical reactions in transition metal complexes substitution, decomposition, rearrangement and redox reactions, applications of photochemical inorganic reactions in synthesis, catalysts, biological processes and inlasers.

Unit IV: Inorganic biochemistry:

Metalloproteins and enzymes – role of metal ions in active sites, structure and functions of metalloproteins and enzymes containing Mg, Ca, V, Mn, Fe, Co, Ni, Cu and Zn ions, detailed structure and mechanistic studies of the following—Mn- photosystem-II, catalase, pseudocatalase, oxygen carriers, haemoglobin, myoglobin, non-porphyrin oxygen carriers, hemerythrin, hemocyanin, Fe-ribonucleotide reductase, cytochrome c oxidases, cytochrome P-450s, hydrogenase, nitrogen fixation, Cu-blue copper protein, tyrosinase, galactose oxidase, superoxide dismutases, Zn-carbonicanhydrase, carboxypeptidase, alcohol dehydrogenase, biological importance of Vitamin B12 and coenzyme.

Unit V: Chemical toxicity and Metallotherapy:

Toxic chemicals in the environment, toxic effects of arsenic, cadmium, lead, mercury, carbon monoxide, cyanide and other carcinogens, metal containing drugs in therapy, interaction of heavy metal ions with DNA, DNA cleavage, structure-activity relationship and mode of action.

Suggested Readings

[l] Huheey, J.E., Keiter, E. and Keiter, R,, "*Inorganic Chemistry: Principles of Structure and Reactivity*", 4th Ed., Pearson Education Asia, 3rd Indian reprint, **2001**.

[3] Wilkins.R.G.,"*Kinetics and Reaction Mechanism of Transition Metal Complexes*", 2nd Revised Ed., VCH, New York,**1991**.

[4] Mukherjee, G.N. and Das, A., "*Elements of Bioinorganic Chemistry*", 1st Ed.. U.N. Dhur & Sons Pvt. Ltd., Calcutta, **1993**.

[5] Lippard, S.J. and Berg, J.,"*Principles of Bioinorganic Chenistry*", University Science Books, U.S.A., **1994.**

7th or 8th Semester

CYE-409: Advanced Methods of Chemical Analysis

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the principles and instrumentation of vibrational spectroscopy, electron spin resonance spectroscopy, NMR spectroscopy, Mossbauer spectroscopy, X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD) techniques.
[CO.2] To learn how to use such techniques in chemical analysis.

Course Objectives:

After completion of the course,
[CO.1] Student(s) will know and understand the principles and instrumentation of vibrational spectroscopy, electron spin resonance spectroscopy, NMR spectroscopy, Mossbauer spectroscopy, X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD) techniques.
[CO.2] Student(s) will learn how to use such techniques in chemical analysis.

COURSE CONTENT

Unit I: Vibrational Spectroscopy

Symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and AB_6, modes of bonding of ambidentate ligands, ethylenediamine and diketonate complexes, application of resonance Raman Spectroscopy particularly for the study of active sites of metalloproteins as myoglobin and haemoglobin.

Unit II: Electron Spin Resonance Spectroscopy

Principle, presentation of the spectrum, hyperfine coupling, hyperfine splitting in various structures, factors affecting magnitude of g, zero field splitting and Kramer's degeneracy, applications to transition metal complexes having one and more than one unpaired electron, applications to inorganic free radicals, study of electron exchange reactions.

Unit III: NMR spectroscopy:

Principle and Instrumentation.

Unit IV: Mossbauer Spectroscopy

Basic principles, spectral display, isomer shift, factors affecting the magnitude of isomer shift, quadrupole and magnetic hyperfine interaction, applications of technique to the study of bonding and structure of Fe^{2+}, Fe^{3+}; Sn^{2+} and Sn^{4+} compounds; detection of oxidation stated nature of M-L bond.

Unit V:

Principles and Applications of XRD and XPS.

Suggested Readings

[1] Drago, R.S., "*Physical Methods in Inorganic Chemistry*", Reinhold Publishing Corp., East West Press.
[2] Graybeal, J. D., "*Molecular Spectroscopy*", McCiraw-Hill, **1988.**
[3] Slichter. C. P., "*Principles of Magnetic Resonance*", Springer Verlag,**1981.**
[4] Banweil, C.N. and McCash, E.L.M.,"*Fundamentals of Molecular Spectroscopy*",4th Ed. McGraw-Hill. 1999.

CYE-410: Frontiers in Bioinorganic Chemistry

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the concepts of bioinorganic chemistry including homeostatic mechanism, metal ion transport, assembly of metalloproteins, role of molybdenum and tungsten in biology, and iron in biosystem

[CO.2] To know and understand the role of metal ions in context of specific diseases, and biominerals

Course Outcomes:

After completion of the course,

[CO.1] Student(s) will be able to know and understand the concepts of bioinorganic chemistry including homeostatic mechanism, metal ion transport, assembly of metalloproteins, role of molybdenum and tungsten in biology, and iron in biosystem

[CO.2] Student(s) will understand the role of metal ions in context of specific diseases, and biominerals

COURSE CONTENT

Unit I: Homeostatic mechanism

Cellular components and pathways in the context of metal ions, homeostatic mechanism in cell - prokaryotes to eukaryotes to human. Evolutionary pathway metals, metallocofactors and prosthetic groups.

Unit II: Metal ion transport and assembly of metalloproteins:

Details of the metal transport in Yeast and in higher organisms, proteins involved in uptake and efflux, assembly of metals in protein, photoactivation, heme synthesis, covalent and non-covalent interactions of heme with protein, assembly of heme in heme proteins- cytochrome c vs cytochrome b5, heme chaperoning and role of CCME, identification of a protein as heme protein, heme oxygenase, reconstitution of hemeproteins with modified heme/other cofactors and their application in biocatalysis and electron transfer.

Unit III: Molybdenum and Tungsten in Biology

Hyperthennophilic and thermophilic bacteria, Mo and W containing enzymes, mechanism of catalytic activity- nitrogenase, sulfite oxidase, nitrate reductase, acetylene hydratase, xanthine oxidase, DMSO reductase, structural and functional modeling of Mo and W sites and their applications as biocatalysis.

Unit IV: Iron in Biosystem

Non-heme-iron-sulphur proteins, other non-heme iron proteins-lipoxygenase and its implication in cancer research, nitrile hydratase and its application to industry, structural and functional modeling of heme and non-heme metal-sites and their applications in biochemistry, heme-catalytic mechanism of nitric oxide synthease and heme oxygenase.

Unit V: Metal Ions and Diseases

Role in Alzheimer's disease- aggregation of proteins, role of copper, zinc and iron, application of radiochemistry for the identification of metal ions, metal binding in prion protein-binding of copper and manganese, manganism- occupational exposure, manganese toxicity, effect on calcium channel, proteomics of manganese toxicity, inorganic NO-donor and their applications.

Unit VI: Biomineralization

Biomineralization in the context of bone, teeth and mollusk cells, application into materials science and biomimetic engineering, bioorganometallic chemistry- introduction and applications.

Suggested Readings

[1] Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M., "*Advanced Inorganic Chemistry*", 6th Ed., John Wiley & Sons, **1999.**

[2] Huheey, J. E., Keiter, E. A. and Keiter, R. L., "*Inorganic Chemistry Principle of Structure and Reactivity*", 4th Ed, Pearson Education, lnc., **2003**.

[3] Mukherjee, G. N. and Das, A., "*Elements of Bioinorganic Chemistry*", U.N. Dhur & Sons Pvt. Ltd., Calcutta, **1993.**

[4] Lippard, S. J. and Berg, J., "*Principles of Bioinorganic Chemistry*", University Science Books, U.S.A., **1994.**

[5] Pecoraro, V. L. "*Manganese Redox Enzymes*", VCH: New York, **1992.**

CYE-411: Inorganic Photochemistry

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the fundamentals of photochemistry
[CO.2] To know and understand the properties of the excited states, excited states of metal complexes
[CO.3] To know and understand the excited states of metal complexes, and ligand-field photochemistry
[CO.4] To know and understand the redox reactions by excited metal complexes, and metal complexes as sensitizers

Course Outcomes:

After completion of the course,
[CO.1] Students will know and understand the fundamentals of photochemistry, the properties of the excited states, and excited states of metal complexes
[CO.2] Students will know and understand the excited states of metal complexes, and ligand-field photochemistry
[CO.3] Students will know and understand the redox reactions by excited metal complexes, and metal complexes as sensitizers

COURSE CONTENT

Unit I: Basics of photochemistry:

Absorption, excitation, photochemical laws, quantum yield, electronically excited states life times-measurements of the times, flash photolysis, stopped flow techniques, energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes.

Unit II: Properties of excited states:

Structure, dipole moment, acid-base strengths, reactivity, photochemical kinetics-calculation of rates of radfative processes, bimolecular deactivation - quenching.

Unit III: Excited states of metal complexes:

Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes, charge-transfer spectra, charge transfer excitations methods for obtaining charge-transfer spectra.

Unit IV: Ligand field photochemistry:

Photosubstitution, photooxidation and photoreduction liability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.

Unit V: Redox reactions by excited metal complexes:

Energy transfer under conditions of weak interaction and strong interaction-exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (,2'-bipyridine and I,10-phennonthroline complexes), illustration of reducing and oxidizing character of Ru(ll)-bipyramidal complex, comparison with Fe(bipy)3; role of orbit coupling- life time of these complexes, application of redox processes of

electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light.

Unit VI: Metal complex sensitizers:

Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation.

Suggested Readings

[1] *Concepts of lnorganic Photochemistry*, A. W. Adamson and P. D. Fleischauer, Wiley.
[2] *Inorganic Photochemistry*. J. Chem. Educ., vol. 60, no. 10, 1983.
[3] *Progress in Inorganic Chemistry*, vol. 30 ed.S. J. Lippard. Wiley.
[4] *Coord. Chem. Rev.*, vol. 39, 121, 131; 1975, 15,321; 1990, 97,313.
[5] *Photochemistry of Coordination Compounds*, V. Balzani and V. Carassiti, Academic Press.
[6] *Elements of lnorganic Photochemistry*. G. J. Ferraudi, Wiley.

CYE-412: Supramolecular Chemistry

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the fundamentals of supramolecular chemistry
[CO.2] To know and understand the role of supramolecular chemistry in biological processes
[CO.3] To learn how to synthesize the supramolecules
[CO.4] To know and understand the physical methods and their use in supramolecular chemistry

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will know and understand the fundamentals of supramolecular chemistry.
[CO.2] Student(s) will know and understand the role of supramolecular chemistry in biological processes.
[CO.3] Student(s) will have the skills to synthesize the supramolecules.
[CO.4] Student(s) will know and understand the physical methods and their use in supramolecular chemistry.

COURSE CONTENT

Unit I: Fundamentals of Supramolecular Chemistry

Definitions, brief overview and examples; types of non-covalent interactions CH-bonding, electrostatic (ion-ion, ion-dipole, dipole-dipole), hydrophobic and steric, pi-pi, van der Waals), concepts of host-guest complexation with examples from ionophore chemistry, complexation of ions, molecular baskets, chalices and cages- podands, crown ethers, cryptands, calixarenes, macrocyclic effect, complexation of neutral molecules, self-assembly, molecular boxes and capsules, self-complementary species and self-replication.

Unit II: Supramolecular Chemistry and Biological Processes

Cation binding (biological relevance, affinity and selectivity, artificial ionophores, natural and artificial cation channels). Anion and neutral molecule binding -relevance factors affecting affinity and selectivity, anion and neutral molecule binding in biology, artificial hosts for anions, katapinands, guanidinium receptors, receptors based upon Lewis's acid-base concepts, enantio-selective anion recogmt10n, cyclodextrins, anion binding based upon ion-dipole interactions, simultaneous anion-cation binding, neutral molecule recognition and binding.

Unit III: Synthesis of Supramolecules

Synthesis of macrocycles, synthesis of receptors for cations anions, and neutral molecules, non-covalent synthesis, metal directed self-assembly of complex supramolecular architecture-rotaxanes, catenanes.

Unit IV: Physical Methods in Supramolecular Chemistry

Spectroscopy in supramolecular chemistry, determination of stoichiometry, stability constants, and geometry of complexes, binding constant determination, dynamics of supramolecular systems (solid state *vs* solution behaviour).

Suggested Readings

[1] Steed, J.W. and Aswood, J.L., "*Supramolecular Chemistry*", Wiley
[2] Dodziuk,,H., "*Introduction to Supramolecular Chemistry*", Springer, ISBN 1402002149.
[3] Beer, P.D., Gale, P.A., Smith, D.K., "*Supramolecular Chemistry*", Oxford Chemistry Printers, ISBN-10: 0-19-850447-0
[4] Cragg, P., "*A Practical Guide to Supramolecular Chemistry*", Wiley-VCH, ISBN: 0-470- 86654-3
[5] Schneider, H.J. and Yatsimirsky, A., "*Principles and Methods in Supramolecular Chemistry*", Wiley-VCR, ISBN: 0-471-97253-3.

CYE-413: Advanced Quantum Chemistry

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the approximate solutions to the Schrodinger equation
[CO.1] To know and understand the electron spin and many electrons-systems
[CO.1] To know and understand the Hartree-Fock Self-Consistent Field method
[CO.1] To know and understand molecular structures, and semiempirical molecular orbital methods I - PI electron systems

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will know and understand the approximate solutions to the Schrodinger equation
[CO.1] Student(s) will know and understand the electron spin and many electrons-systems
[CO.1] Student(s) will know and understand the Hartree-Fock Self-Consistent Field method, molecular structures, and semiempirical molecular orbital methods I - PI electron systems

COURSE CONTENT

Unit 1: Introduction

Vector Interpretation of Wave function, Hermitian Operator, The Generalized Uncertainty principle, The quantum Mechanical Virial Theorem, Solution of harmonic oscillator (Operator approach), Second quantization (Boson and Fermion), Quantum theory of angular momentum, One electron Atom, Spin angular momentum.

Unit 2: Approximate solutions to the Schrodinger Equation:

The Variation method (Time independent and Time Dependent), Time independent perturbation theory (non – degenerate and degenerate), Time dependent perturbation theory.

Unit 3: Electron Spin and Many - Electron Systems

The Antisymmetry Principle, Spin angular momenta and their Operators, The Orbital Approximation (Slater determinant, Pauli exclusion principle), Two electron wave functions.

Unit 4: The Hartree-Fock Self-Consistent Field Method

The generation of Optimized orbitals, Koopman's Theorem (The Physical Significance of Orbital Energies), The electron correlation energy, Density matrix analysis of the Hartree-Fock Approximation, Natural orbitals, The matrix solution of the Hartree- Fock Equations (Roothaan's equations).

Unit 5: Introduction to Molecular Structure

The Born - Oppenheimer Approximation, Solution of the Nuclear Equation, Molecular Hartree- Fock Calculations. Electronic Structure of Linear Molecule: The MO - LCAO Approximation, The Hydrogen Molecule Ion, H_2^+, The Hydrogen molecule, Molecular Configuration - Interactions, The Valence Bond Method, Molecular Perturbation Calculations. Electronic Structure of Non-linear Molecule: The AHn molecule: Methane, Ammonia and Water, Hybrid Orbitals: The Ethylene and Benzene Molecules.

Unit 6: Semiempirical Molecular Orbital Methods I - PI Electron Systems

The Huckel Approximation for Conjugated Hydrocarbons, The Pariser-Parr-Pople Method. Semiempirical Molecular Orbital Methods II - All valence – Electron systems: The Extended Huckel Method, The CNDO Method.

Suggested Readings

[1] Levine, I. N. "*Quantum Chemistry*", 7th Ed., PHI Learning Pvt. Ltd., Delhi.
[2] McQuarrie, D. A. "*Quantum Chemistry*" Reprint, Viva Books.
[3] Atkins, P. "*Molecular Quantum Mechanics*", 4th Ed., Oxford University Press.
[4] Cotton, F. A., "*Chemical Applications of Group Theory*", Reprint, Wiley Eastern
[5] Banwell, C.N. and McCash, E.L.M.,"*Fundamentals of Molecular Spectroscopy*", 4th Ed. McGraw-Hill N. Y.
[5] Slichter, C.P., "*Principles of Magnetic Resonance*", Springer Verlag.
[6] Graybeal, J.D., "*Molecular Spectroscopy*", McGraw-Hill.

CYE-414: Chemistry of Natural Products

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the chemistry of natural products such as lignin, pectins, carbohydrates, terpenoids, pyrethroids and rotenoids
[CO.2] To know and understand the pathways of the oxidation of carbohydrates
[CO.3] To know and understand the biosynthesis of natural products

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will know and understand the chemistry of natural products such as lignin, pectins, carbohydrates, terpenoids, pyrethroids and rotenoids
[CO.2] Student(s) will know and understand the pathways of the oxidation of carbohydrates
[CO.3] Student(s) will know and understand the biosynthesis of natural products

COURSE CONTENT

Natural coloring matter, general classification, method of synthesis, biosynthesis studies of carotenoids (β-carotene), anthocyanins (cyanine), flavones (chryosin) and flavanol (Querecetin).
Porphyrin-structure, spectral properties and synthesis, general and structure determination of Haemoglobin. chlorophyll and Bilirubin.

Unit I: Lignin and Pectins

Lignin: Chemical composition, structure, functions and chemistry.
Pectins: Chemical composition, structure, chemistry and commercial utilization.

Unit II: Carbohydrates and their Biological Oxidation

Classification of carbohydrates, reducing and non-reducing saccharides, D & L notations, Epimers, mutarotation and anomers.
Oxidation to Pyruvate: Glycolysis, Entner-Duodorf (ED) pathway, phosphoketolase pathway; aerobic pathways: Krebs citric acid cycle, electron transport. Fermentations: alcohol and lactic acid.

Unit III: Terpenoids

Classification, nomenclature, general methods of structure determination, chemistry and synthesis of abietic acid and gibberellic acid (gibberllin-A), farnesol, zingeberine and squalene) Biosynthetic studies on triterpenoids and tetraterpenoides.

Unit IV: Pyrethroids and Rotenoids

Classification, nomenclature, general methods of structure determination, chemistry and toxicity of synthetic pyrethroids and rotenoids.

Unit IV: Biosynthesis of Natural Products

Biosynthesis of carbohydrates (glucose), steroids (cholesterol) and alkaloids (tropane, isoquinoline, indole).

Suggested Readings

[1] Finar, I. L. (1956). Organic Chemisfly, Volume 2: Stereochemistry and The Chemistry Natural Products, 5th Ed. Pearson Education India.
[2] Singh, J.; Ali, S.M. & Singh, *J. Natural Product Chemistry,* Prajati Parakashan 2010.
[3] Agarwal, O. P. *Chemistry of Organic Natural Products, Vol 1 and 2,* Goel Pub. House, 2002.
[4] Chatwal, Gurdeep. *Chemistry of Organic Natural Products, Vol 1 and 2,* Goel Pub. House, 2002
[5] Cooper, R., & Nicola, G. (2014). Natural Products Chemistry: Sources, Separations and Structures. CRC Press.
[6] Schaefer, B. (2015). *Natural products in the chemical industry.* Springer.
[7] Siddiqui A.A., Siddiqui S. *Natural Products Chemistry Practical Manual,* CBS Publishers.

CYE-415: Organic Structure Determination

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the fundamentals and applications of UV-Vis, infrared (IR) and 1D-NMR spectroscopic and mass spectroscopic techniques in the structure elucidation of organic compounds

[CO.2] To know and understand the principles and applications of 2D-NMR spectroscopic techniques in the structure elucidation

Course Outcomes:

After completion of the course,

[CO.1] Learners will have the skills to interpret the data of UV-Vis, infrared (IR) and 1D-NMR spectroscopic and mass spectroscopic techniques.

[CO.2] Learners will know and understand the fundamentals and applications of UV-Vis, infrared (IR) and 1D-NMR spectroscopic and mass spectroscopic techniques.

[CO.3] Learners will have the skills to apply the spectroscopic techniques in the structure elucidation of organic compounds.

[CO.4] Learners will know and understand the principles and applications of 2D-NMR spectroscopic techniques in the structure elucidation.

COURSE CONTENT

Unit I: Electronic Spectroscopy

Electronic transitions in organic molecules, Woodward-Fieser rules for alkenes, Woodward rules for enones, aromatic compounds.

Unit II: Infrared and Raman spectroscopy

For simple organic molecules, predicting number of active modes of vibrations, analysis of representative spectra of compounds with various functional groups, application of isotopic substitution.

Unit III: Mass Spectrometry

Basic principles, hard and soft ionization techniques, mass analyzer in ESI-MS and MALDT MS, high resolution MS, isotope abundance, molecular ion, fragmentation processes (McL) of organic molecuJes, deduction of structure through mass spectral fragmentation.

Unit IV: Nuclear Magnetic Resonance

Effect of magnetic field strength on sensitivity and resolution, chemical shift 8, inductive and anisotropic effects on 6, chemical structure correlations of 8, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant *J*, first order and second order spectra, examples of AB, AX, ABX, AMX and AA'BB' systems, simplification of second order spectrum, selective decoupling, double resonance, use of chemical shift reagents for stereochemical assignments, ^{13}C NMR, Tl relaxation, NOE effects, DEPT, determination of number of attached hydrogens, ^{1}H and ^{13}C chemical shifts to structure correlations, study of dynamic processes by VT NMR. restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (fulvalene and related systems). Multinuclear NMR, COSY, DQF-COSY, HETCOR, HMQC, HMBC, TOCSY, ROESY, VGSE.

Unit V: Spectroscopic Application

Structure elucidation of organic compounds using spectroscopic methods.

Suggested Readings

[1] Silverstein, R. M., Webseter, F. X. and Kiemle, D., *"Spectrometric Identification of Organic Compounds"*, 7th Ed., John Wiley &Sons.
[2] Kemp, W. L., *"Organic Spectroscopy*", Palgrave.
[3] Pavia, D. L., *"Spectroscopy"*,4th Ed., Cengage.
[4] Williams, D. and Fleming, l., *"Spectroscopic Methods in Organic Chemistry"*, 6th Ed., McGraw Hill Education (India) Private Limited.

CYE-416: Modern Organic Synthesis Methods

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the various types of oxidation reactions
[CO.2] To know and understand the modern reactions of high utility in organic synthesis
[CO.3] To learn how to protect and deprotect the functional groups during multistep organic synthesis
[CO.4] To know and understand the retrosynthetic approach

Course Outcomes:

After completion of this course,
[CO.1] Students will know and understand the various types of oxidation reactions
[CO.2] Students will know and understand the modern reactions of high utility in organic synthesis
[CO.3] Students will know how to protect and deprotect the functional groups during multistep organic synthesis
[CO.4] Students will know and understand the retrosynthetic approach

COURSE CONTENT

Unit I: Oxidations

Oxidations of hydrocarbons (alkanes, alkenes and aromatic), alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation, alkenes to diols (Manganese, Osmium-based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, alkenes to carbonyls with bond cleavage (manganese, osmium, ruthenium and lead based-ozonolysis), alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation), ketones to α-hydroxy ketones, α,β-unsaturated ketones, ester/lactones (Baeyer-Villiger), alcohols to carbonyls (chromium, manganese, aluminum, silver, ruthenium, DMSO, hypervalent iodine and TEMPO based reagents), alcohols to acids or esters, phenols (Fremy's salt, silver carbonate).

Unit II: Named reactions

Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction, Brook rearrangement and Tebbe olefination.

Unit III: Protection and Deprotection of Functional Groups

Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds, chemo- and regioselective protection and deprotection, illustration of protection and deprotection in multi-step synthesis.

Unit IV: Retrosynthetic analysis:

Basic principles and terminology of retrosynthesis, guidelines, synthesis of aromatic compounds, one group and two group C−X disconnections, one group C−C and two group C−C disconnections, amine and alkene synthesis, important strategies of retro synthesis, functional group transposition, important functional group interconversions, reversal of polarity (umpolung).

Suggested Readings

[1] Carey, F. A. and Sundberg, R. J., *"Advanced Organic Chemistry, Part B: Reactions and Synthesis"*, 5th Ed., Springer.
[2] Carruthers, W. and Coldham, I., *"Modern Methods of Organic Synthesis"*, 4th Ed., Oxford University Press.
[3] Smith, M.B., *"Organic Synthesis"*, 3rd Ed., Academic Press.
[4] Stuart "*Organic Synthesis*"

CYE-417: Medicinal Chemistry

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the drugs, and intermolecular interactions
[CO.2] To know and understand the drug targets including proteins, enzymes and receptors, their structures and functions
[CO.3] To know and understand the concepts of pharmacokinetic and pharmacodynamics, the enzymes as drug targets, receptors as drug targets, and nucleic acids as drug targets
[CO.4] To know and understand the drug discovery, design, development, identification of the structure–activity relationships (SARs), and the pharmacophore in the drug design, and the ways to improve target interactions (pharmacodynamics) and improve pharmacokinetic properties.
[CO.5] To know and understand the preclinical trials and significance of patent on the drug

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will know and understand the drugs, and intermolecular interactions.
[CO.2] Student(s) will know and understand the drug targets including proteins, enzymes and receptors, their structures and functions.
[CO.3] Student(s) will know and understand the concepts of pharmacokinetic and pharmacodynamics, the enzymes as drug targets, receptors as drug targets, and nucleic acids as drug targets.
[CO.4] Student(s) will know and understand the drug discovery, design, development, identification of the structure–activity relationships (SARs), and the pharmacophore in the drug design, and the ways to improve target interactions (pharmacodynamics) and improve pharmacokinetic properties.
[CO.5] Student(s) will understand the preclinical trials and significance of patent on the drug.

COURSE CONTENT

Unit I:
An introduction to drugs, drug targets and intermolecular interactions
Unit II: Drug targets
Protein: structure and function
Enzymes: structure and function
Receptors: structure and function
Unit III: Pharmacokinetic and Pharmacodynamic
Enzymes as drug targets, receptors as drug targets, nucleic acids as drug targets
Unit IV: Drug Discovery, Design, and Development
Finding a lead: choose a disease, choose a drug target, identify a bioassay, find a 'lead compound', isolate and purify the lead compound, determine the structure of the lead compound if necessary.
Drug design: Identify structure–activity relationships (SARs), identify the pharmacophore, improve target interactions (pharmacodynamics), improve pharmacokinetic properties.
Drug development: patent the drug, carry out preclinical trials (drug metabolism, toxicology, formulation and stability tests, pharmacology studies, etc.)

Suggested Readings

[1] *An introduction to medicinal chemistry*, Graham Patrick, Oxford University Press, UK, 2013.
[2] *The Organic Chemistry of Drug Design and Drug Action*, Rchard Silverman, Academic Press.
[3] *Medicinal Chemistry: A Molecular and Biochemical Approach*, Thomas Nogrady and Donald F. Weaver
[4] *Burger's Medicinal Chemistry and Drug Discovery* 6 Volume Set March 2003, Wiley ISBN Number 0-471-37032-0.

CYE-418: Solid State Chemistry and Applications

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the crystal structures of inorganic compounds, and defect structures
[CO.2] To learn how to synthesize solid state materials.
[CO.3] To know and understand amorphous inorganic materials, intercalation chemistry.
[CO.4] To know the use of physical methods in the structural characterization of metal complexes.

Course Outcomes:

After completion of the course,
[CO.1] Students will know and understand the crystal structures of inorganic compounds, and defect structures.
[CO.2] Students will know how to synthesize solid state materials
[CO.3] Students will know and understand amorphous inorganic materials, intercalation chemistry
[CO.4] Students will know and understand the use of physical methods in the structural characterization of metal complexes.

COURSE CONTENT

Unit I: Crystal structure of inorganic compounds

Overview of close packing, packing efficiency, interstitial sites, limiting radius ratios, method of determination of ionic radii. Ionic crystals containing two or three different elements– FeO, ZnO, CdS, fluorite, antifluorite, nickel-arsenide, CaC_2, CdI_2 and TiO_2, $FeTiO_3$, $MgAl_2O_4$, Fe_2NiO_4, garnets, $BaTiO_3$ and $KNiF_3$. Non-ionic crystals– SiC, (BN)x, giant molecules, layer structures, crystals composed of discrete molecules.

Unit II: Defect structures

Thermodynamic defects and their consequences, solid electrolytes, non-stoichiometric compounds, F-centers and applications of defects in non-stoichiometric compounds.

Unit III: Methods to synthesize solid-state materials

Ceramic method, solid-state reaction and its kinetics, hydrothermal, sol-gel, co-precipitation (precursor), vapour phase transport methods. Different methods to grow single crystals.

Unit IV: Amorphous Inorganic Materials

Glasses, refractories, materials obtained from organometallic chemical vapour deposition (MOCVD). New materials: Conducting polymers, carbon nanotubes, carbon nanorods and fullerenes. Electronic materials: Insulating, semiconducting and superconducting materials, ferroelectrics and dielectrics.

Unit V: Intercalation chemistry

Introduction, intercalation reactions in graphite, layered double hydroxides, layered sulfides, applications of intercalation chemistry. Mesoporous materials and their catalytic applications: Various types of mesoporous materials (oxides, sulphides), tailoring of pore size, applications of mesoporous materials in heterogeneous catalysis.

Unit VI: Structural Characterization of Metal Complexes by Physical Methods

Extended X-ray absorption spectroscopic (EXAFS), X-ray photoelectron spectroscopic (XPS), X-ray absorption near edge spectroscopic (XANES), electron spin spectrometric (ESR), electron

spectroscopy for chemical analysis (ESCA) studies, soild state NMR, HMBC, HMQC, Mössbauer spectroscopic studies of metal complexes, thermal methods (TG, DTA and DSC), atomic force microscopy (AFM) and transmission electron microscopy (TEM).

Suggested Readings

[1] Douglas, B.E., McDaniel, D.H. and Alexander, J.J., "*Concepts and Models of Inorganic Chemistry*", 3rd Ed., John Wiley & Sons, Inc., New York.

[2] West, A.R., "*Solid State Chemistry and its Applications*", Reprint, Wiley India.

[3] Smart, L. and Moore, E., "*Solid State Chemistry: An Introduction*", Nelson Thornes Ltd.

[4] Rao, C.N.R. and Gopalakrishnan, J. "*New Directions in Solid State Chemistry*", 2nd Ed., Cambridge University Press, Cambridge.

CYE-419: Advanced Surface and Colloidal Chemistry

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the surfactants and interfacial phenomena, and thermodynamics of surfaces and interphases

[CO.2] To know and understand the membranes and their applications

[CO.3] To understand the adsorption on solids/porous materials, and colloid systems and their properties

Course Outcomes:

After completion of the course,

[CO.1] Student(s) will know and understand the surfactants and interfacial phenomena, and thermodynamics of surfaces and interphases.

[CO.2] Student(s) will know and understand the membranes and their applications.

[CO.3] Student(s) will know and understand the adsorption on solids/porous materials, and colloid systems and their properties.

COURSE CONTENT

Unit I: Surfactants and Interfacial Phenomena

Classification, micellization, c.m.c. and its determination. Shape and structure of micelles, effect of additives on micellization, thermodynamics of micellization, solubilization and applications, effect of electrolytes on solubilization. Macro and micro emulsions, dispersion and aggregation of solids by surfactants.

Unit II: Thermodynamics of Surfaces and Interphases:

Surface and interfacial phenomenon, macromolecules, adsorption of gases by solids, BET theorem, determination of surface area of solids, adsorption from solution, electrical phenomenon of interphases. electrode- solution interface, rate of charge transfer in electrode reactions,

Unit III: Membranes and their Applications

Artificial and natural membranes, Donnan membrane equilibrium, transport of electrolytes, membrane potential and ion selective electrodes.

Unit IV: Adsorption on solids and porous materials

Model for multilayer adsorption, BET isotherm and application to different types of adsorbents, adsorption by porous, non-porous and microporous solids. Estimation of specific surface area and pore size distribution. Special problems encountered with very narrow pore size material and adsorption from liquid phase.

Unit V: Colloid systems and their properties

Origin of the charges, electro-kinetic phenomena, electrophoresis, electro-osmosis, sedimentation and streaming potential. The concept of electrical double layer and various models to explain its structure and properties, DLVO theory and stability of colloids. Smoluchowski theory of kinetics of coagulation and distribution of colloids aggregates. Organic and inorganic gels and clay colloids.

Suggested Readings

[1] Hunter, R. J., "*Foundation of Colloid Science*", Oxford Univ. Press.
[2] Lyklema, J., "*Fundamentals of Interface and Colloid Science*", Academic Press San Diego.
[3] Adamson, A.W.,"*Physical Chemistry of Surfaces*", 5th Ed., John Wiley and Sons, New York.
[4] Kruyt, H.R., "*Colloid Chemistry*" Vol. I & II. Elsevier Press.
[5] Greg, S.J. and Singh, K.S.W., "*Adsorption, Surface Area and Porosity*", 2nd Ed., Academic Press. U K.
[6] Flory P. J., "*Principles of Polymer Chemistry*", 1st Ed., Cornell University Press.
[7] Rubinstein M. and Colby R. C., "*Polymer Physics*", 1st Ed., Oxford University Press.
[8] Billmeyer, F. W., "*Textbook of Polymer Science*", 3rd Ed., Wiley India Private Limited.

CYE-420: Environmental Pollutants and Analysis

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the environmental chemistry of water, water pollution, water treatment options, advanced waste water treatment, analysis of major constituents/common ions/trace pollutants in water

[CO.2] To know and understand the atmosphere, atmospheric Chemistry, air pollutants, organic air pollutants, and atmospheric analysis of gases/particulates

[CO.3] To know and understand the formation, properties, and analysis of soils

[CO.4] To know and understand the toxicological chemistry, and fate of hazardous wastes.

Course Outcomes:

After completion of the course,

[CO.1] Students will know and understand the environmental chemistry of water, water pollution, water treatment options, advanced waste water treatment, analysis of major constituents/common ions/trace pollutants in water.

[CO.2] Students will know and understand the atmosphere, atmospheric Chemistry, air pollutants, organic air pollutants, and atmospheric analysis of gases/particulates.

[CO.3] Students will know and understand the formation, properties, and analysis of soils .

[CO.4] Students will know and understand the toxicological chemistry, and fate of hazardous wastes.

COURSE CONTENT

Unit I: Introduction

Environmental Segments (Atmosphere, Hydrosphere, Lithosphere, Biosphere), Natural Cycles of the environment (The Hydrologic, Oxygen, Nitrogen, Phosphate and Sulphur Cycle), Commonly Used Terms

Unit II: Environmental Chemistry of Water

Properties of water, The Characteristics Of Bodies Of Water, Alkalinity of water, Source and nature of acidity, Major aquatic chemical processes, Oxidation - reduction reactions in water, pE-pH diagram, Complexation, Redox Reactions Mediated By Bacteria, Nitrogen Transformation by Bacteria

Water Pollution

Synthetic Organic pollutants, Soaps and Detergents, Pesticides, Polychlorinated dibenzodioxins (PCDDs) and Polychlorinated Dibenzofurans (PCDFs), Polychlorinated Biphenyls, Elemental Pollutants, Other inorganic pollutants, Eutrophication and Algal Nutrients, Acid Mine drainage, Accumulation of Salts in water, Oxygen sag curve, Regulation of water quality, Secondary standards

Water Treatment Operations

Municipal water treatment for raw water, Treatment of raw water for industrial use, Waste Water Treatment, Basic processes of water treatment, Primary treatment of waste water, Secondary treatment for municipal waste water, Trickling filters, Rotating biological contactor, Activated sludge process, The significant processes that occur in biological waste treatment, Oxidation ponds.

Advanced Waste Water Treatment

Removal of Suspended Solids Removal of dissolved solids, Phosphate removal (chemical treatment) Phosphate removal (biological treatment), Removal of dissolved organic compounds,

Analysis of Major Constituents in Water

Water Sampling and Storage, Water Quality Measurement, Oxygen demand pH, Acidity and Alkalinity

Analysis of Common Ions at Low Concentrations in Water

Ultraviolet and Visible Spectrometry, Spectrophotometric instrumentation, Analysis by direct absorption, Analysis after formation of derivative, Examples of The Use Of Other Techniques.

Analysis of Trace Pollutants in Water

Bio Concentration, Accumulation in sediments, Biomagnification, Degradation, Gas liquid Chromatography (GC) Detectors, Extraction procedures or sample preparation, High Performance Liquid Chromatography (HPLC), Analysis of Metal Ions present at trace levels, Sample containers and storage, Chelation ion liquid chromatography, Speciation of Chromium by ion chromatography, Mass spectrometric detector for GC for the determination of ultratrace levels of (ngL^{-1}) polychlorinated organic compounds

Unit III: The Atmosphere and Atmospheric Chemistry

Importance of the atmosphere, Physical characteristics of the atmosphere, Major regions of the atmosphere, Evolution of the atmosphere, Earth's Radiation, Balance Carbon Dioxide In the atmosphere, Water vapour in the atmosphere, Ions and radicals in the atmosphere, Reactions involving hydroxyl and hydroperoxyl radicals, Atmospheric reactions of oxygen, Atmospheric reactions of nitrogen.

Air Pollutants

Carbon Oxides, Sources of CO pollution, Carbon Dioxide and Global Warming, Sulphur Dioxide: Sources and Removal, Nitrogen oxides in the atmosphere, Acid rain, Particles in the atmosphere.

Organic Air Pollutants

Natural source of hydrocarbons, Oxygen-containing organic compounds, Organohalide compounds, Chlorofluow carbons and depletion of ozone layer, CFC substitutes, Consequences of ozone depletion, Photo chemical smog, Chemical reactions involved in smog formation in the atmosphere, Organo nitrogen compounds, Organic particles in the atmosphere, Nitrogen oxides in the atmosphere, Acid rain, Particles in the atmosphere.

Atmospheric Analysis of Gases

Introduction Determination oftime-weighted average concentrations, Determination of inorganic gaseous pollutants, Determination low-concentrations of organic pollutants, Desorption of the analyte, Determination of instantaneous concentrations, Chemiluminescence and fluorescence, Infrared spectrometry for carbon monoxide, Electrochemical sensors minimization, Gas detector tubes, Gas solid chromatography, Sampling, Gas-solid chromatographic analysis.

Atmospheric Analysis of Particulates

Measurement and Characterisation of the particulate content, Sampling methods, Determination of totaJ organic content in the gas sample, Analysis of particulates after dissolution, Direct analysis of particulates, Drawbacks of the direct analysis.

Unit IV: Soil

Soil Formation and Properties

Introduction, Kinds of Rocks and Formation of Soil, Mineral components in soil. Exchangeable cations and cation exchange capacity, Acid - Base ion exchange reaction in soils, Profile and Its Importance, Micro and macro-nutrients in soil, Nitrogen phosphorous and potassium in soil, Wastes and pollutants in soil.

Analysis of Soils, Sediments and Biological Specimens

Sampling, Sample Preparation, Extraction of the analyte and determination, Sample preparation, Plant materials, biological tissues and fluids.

Unit V: Toxicological Chemistry

Toxic chemicals and toxicity, Kinetic phase and dynamic phase, Physiological responses to toxicants, Teratogenesis, mutagenesis and carcinogenesis, Toxicity of metals, inorg. compounds & org. compounds, Toxicity of some inorganic compounds

Toxicology of Some Organic Compounds

Benzene formaldehyde & acetaldehyde, polycyclic aromatic hydrocarbons (PAHs), phenols, Nitrosamines, lsocyanates and methyl isocyanates, Organophosphates and arbates, Inhibition by carbamate insecticide, Organochlorine compounds & PCBs, Dioxins andpolychlorinated biphenyls, Polychlorinated biphenyls

Unit VI: Reactions and Fate of Hazardous Wastes

Segregation of hazardous wastes, Transport of hazardous wastes, Reactions of hazardous waste

Hazard Waste Reduction and Minimisation and Physical Methods of Treatment of Hazardous Wastes:

Hazardous waste treatment technologies, Physical treatment methods

Chemical Methods of Treatment of Hazardous Wastes

Chemical oxidation and reduction, Ozonolysis, Acid-base neutralization, Chemical precipitation, Hydrolysis, Ion exchange, Thermal treatment methods, Performance of hazardous wastes incinerators, Advantages of incineration, Disadvantages of incineration, Wet air oxidation, Photolysis, Biological treatment of hazardous wastes, Land treatment, Preparation of wastes for disposal.

Suggested Readings

[1] Aland Wild., *Soils and the environment*, Cambridge University Press, New York, 1993.
[2] De., A.K., *Environmental Chemistry*, 4th ed., New Age international (P) Limited, New Delhi 2001.
[3] Fifield, F.W., and P.J. Hains., *Environmental Analytical Chemistry*, 1st ed., Blackie Academic and Professional, Glasgow, UK, 1995.
[4] Gary W. Vanloon., and Stephen J. Duffy., *Environmental chemistry, a global perspective*, Oxford university press, New York, 2000.
[5] Gerard Kiely., *Environmental Engineering*, Irwin Mc Graw-Hill, UK, 1998.
[6] Gilbert M. Masters., "*Introduction to Environmental Engineering and Science*" Prentice Hall of India (Private) Ltd., New Delhi, 1994.
[7] J. Jeffrey Peirce., Ruth F. Weiner and P. Aame VesiliJ1d., *Environmental Pollution and control*, 4th ed.,Butterworth-Heinemann, Woburn, MA,1998.
[8] John P. Hager., Barry J. Hansen., John F. Pusateri., William P. Imrie., and V. Ramachandran., *Extraction and Processing for the treatment and minimization of Wastes*, The Minerals, metals and Materials society., Pennsylvania, 1994.
[9] Loconto, Paul R, *Trace environmental quantitative analysis*, Taylor and Francis, 2006.
[10] Michael D. Lagrega., Philip L. Buckingham., and Jeffrey C. Evans., *Hazardous Waste Management*, Mc Graw-Hill, inc. New York, 1994.
[11] Peter O' Neill., *Environmental Chemistry*, George Allen & Unwin (Publishers) Ltd, London, UK, 1985.
[12] Pradyot Patnaik., *Handbook of Environmental Analysis*, CRC Press, Boca Raton, Florida, 1997.
[13] Rao. C.S., *Environmental Pollution Control Engineering*, New Age International (P) Limited, New Delhi, 1991.
[14] Roger N. Reeve., and John D. Barnes., *Environmental Analysis*, John Wiley & sons, Chichester, UK, 1994.
[15] Stanley E. Manahan., *Environmental Chemistry*, 8th Ed., CRC Press LLC, Boca Raton, Florida, 2005.
[16] Thomas G. Spiro., and William M. Stigliani., 2nd ed., Prentice Hall of India (P) Ltd., New Delhi, 2003.
[17] Vladmir N. Bashkin., *Environmental Chemistry: Asian Lessons*, Kluwer Academic Publishers, Dordrecht, The Netherlands, 2003.
[18] William F. Pickering., *Pollution Evaluation, the quantitative aspects*, Marcel Dekker, New York, 1977.

CYE-421: Macromolecules and Nanomaterials

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the surfactant aggregation
[CO.2] To know and understand the functional polymers
[CO.3] To know and understand the nanomaterials

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will know and understand the surfactant aggregation, and functional polymers
[CO.2] Student(s) will know and understand the historical perspective, effects of nanoscience and nanotechnology on various fields, and synthesis & characterization of nanoparticles.

COURSE CONTENT

Unit I: Surfactant Aggregation:

Micelles**,** Surface active agents, Classification of surface-active agents, Micellization, Hydrophobic interaction, Critical micellar concentration (cmc), Factors affecting concentration of surfactants, Counter-ion binding of micelle, Thermodynamics of micellization, Phase separation and Mass action models, Solubilization Emulsions, Mechanism of fonnation of microemulsion and their stability, Physical techniques, Applications.

Unit II: Functional Polymers:

Smart materials -uses of smart materials in sensing devices and communication networks, conducting polymers: Electrically conducting polymers and their uses. Photoconductive polymers. Liquid crystal polymers - smectic, nematic and cholesteric structures. Ionic exchange polymers: Cationic and anionic exchange polymers and their uses. Eco- friendly polymers, Membrane separation. Filtration- micro, ultra and nanofiltration. Liquid separation- dialysis, electro osmosis and reverse osmosis, Fire retarding polymers, photonic polymers. fnter penetrating networks (IPN), polymers, Polymers in biomedical applications - artificial organs and controlled drug delivery.

Unit III: Nanomaterials:

Definition, historical perspective and effects of nanoscience and nanotechnology on various fields. Synthesis of nanoparticles by chemical routes and characterization techniques: Thermodynamics and kinetics of nucleation; Growth of polyhedral particles by surface reaction, Ostwald ripening, size distribution; TEM; SEM; AFM; Light scattering; *XPS*. Properties of nanostructured materials: Preparation by sol-gel and hydrothermal methods, Optical properties; magnetic properties; chemical properties. Overview of applied chemistry of Nanomaterials.

Suggested Readings

[1] G. C. Bond, *Principles of Heterogeneous Catalysis in practice*, Oxford Publishing.
[2] C. Satterfield, *Heterogeneous Catalysis*, McGraw Hill
[3] *Catalysis, Principles and applications*, edited by B. Vishwanathan, S. Sivasanker & A. V.
[4] *Textbook of Polymer Science*, F. W. Billmeyer Jr, John Wiley & sons
[5] *Polymer Science*, V. R. Gowarikar, N. V. Viswanathan&**J.** Sreedhar, Wiley Eastern
[6] *Contemporary Polymer Chemistry*, H.R. Alcock& F. W. Lambe, Prentice Hall
[7] *Physics and Chemistry of Polymers*, J.M. G.Cowie, Blackie Academic and professional
[8] *Introduction to polymer Chemistry*, By Charles E Carraher Jr (Taylor- Frncis)
[9] *Solid State and its Applications* by A.R. West.
[10] *New directions in solid state chemistry*, J. Gopalakrislman and C.N. R. Rao.
[11] *Principles of the solid state* by HV Keer

CYE-422: Green Methods of Synthesis

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the need and principles of green chemistry
[CO.2] To know and understand the methods for green syntheses of organic compounds
[CO.3] To know and understand the use of microwaves and ultrasound in green syntheses
[CO.4] To know and understand the future trends in green chemistry

Course Outcomes:

After completion of the course,
[CO.1] Student(s) will know and understand the need and principles of green chemistry
[CO.2] Student(s) will know and understand the methods for green syntheses of organic compounds, and the use of microwaves and ultrasound in green syntheses
[CO.3] Student(s) will know and understand the future trends in green chemistry

COURSE CONTENT

Unit I: Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

Unit II: Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/ minimization of hazardous/ toxic products; designing safer chemicals - different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization - careful use of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Unit III: Examples of Green Synthesis/ Reactions

1. ***Green Synthesis of the Compounds:*** such as adipic acid, catechol, BHT, methyl methacrylate, urethane, aromatic amines (4-aminodiphenylamine), benzyl bromide, acetaldehyde, disodium iminodiacetate (alternative to Strecker synthesis), citral, ibuprofen, paracetamol, furfural.

2. ***Microwave Assisted Reactions in Water:*** Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzole acid), Oxidation (of toluene, alcohols).
   Microwave Assisted Reactions in Organic Solvents: Esterification, Fries rearrangement, Orthoester Claisen Rearrangement, Diels-Alder Reaction, Decarboxylation. *Microwave Assisted Solid State Reactions:* Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles from aldehydes; anhydrides from dicarboxylic acid; pyrimidine and pyridine derivatives; 1,2-dihydrotriazine derivatives; benzimidazoles.

3. ***Ultrasound Assisted Reactions:*** Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizaro reaction, Strecker synthesis, Reformatsky reaction.

4. **Selective Methylation of Active Methylene Group using Dimethylcarbonate:** Solidstate polymerization of amorphous polymers using diphenylcarbonate; Use of "Clayan", a nonmetallic oxidative reagent for various reactions; Free Radical Bromination; Role of Tellurium in organic syntheses; Biocatalysis in organic syntheses.

Unit IV: Future Trends in Green chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; oncovalent derivatization; Green chemistry in sustainable development.

Suggested Readings

[1] A.S. Matlack: *Introduction to Green Chemistry*, Marcel Dekker (2001).
[2] V.K. Ahluwalia & M.R. Kidwai: *New Trends in Green Chemistry*, Anamalaya Publishers (2005).
[3] P.T. Anastas & J.K. Warner: Oxford *Green Chemistry-Theory and Practical*, University Press (1998).
[4] M.C. Cann & M.E. Connely: *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).

CYE-423: Total Organic Synthesis

(Discipline Specific Elective Course for the students of 7th or 8th Semester)

Type	:	Elective Course
Total Credits	:	04 (Theory: 4 + Practical: 0)
Total Hours	:	60 Theory + 0 Practicals
Lectures	:	04 per week
Tutorial	:	0
Practical	:	0

Course Objectives:

[CO.1] To know and understand the strategies for synthesis of complex molecular architectures
[CO.2] To know and understand the total synthesis of antibiotics, alkaloids, and terpenoids.
[CO.3] To know and understand the total synthesis of steroids and hormones.

Course Outcomes:

After completion of this course,
[CO.1] Students understand the strategies for synthesis of complex molecular architectures.
[CO.2] Students will know and understand the total synthesis of antibiotics, alkaloids, and terpenoids.
[CO.3] Students will know and understand the total synthesis of steroids and hormones.

COURSE CONTENT

[1] Introduction to strategies for synthesis of complex molecular architectures.
[2] Synthesis of antibiotics - penicillin V and tetracycline.
[3] Synthesis of alkaloids - reserpine and camptothecin.
[4] Synthesis of terpenoids - β-pinene, camphor, abietic acid and β-amirine.
[5] Synthesis of steroids and hormones - cholesterol, progesterone and cortisone
[6] Synthesis of prostaglandins PGE_2 and PGF2α; glycosidic pigments anthocyanins and quercetin; macrocyclic lactam fluvirucin-B1-aglycone; and vitamin biotin.

Suggested Readings

[1] Finar, I.L., *"Organic Chemistry"*, Vol .2, 5th Ed., ELBS
[2] Corey, E.J. and Cheng, X.-M., *"The Logic of Chemical Synthesis"*, Wiley-VCH, Weinheim
[2] Nicolaou, K.C. and Sorensen, E.J., *"Classics in Total Synthesis"*, Wiley-VCH, Weinheim
[4] Gewert, J.A., Gorlitzer, J., Gotze, S., Looft, J, Menningen, P., Nobel, T., Schimek, H. and Wulff, C., *"Organic synthesis workbook'*, Wiley-VCH, Weinheim.