

5-Year Integrated M.Sc. in Chemistry
[Exit Option after 03 Years with B.Sc. (Hons.) Degree in Chemistry]

Applicable July 2018 Onwards

CURRICULUM



DEPARTMENT OF CHEMISTRY
SCHOOL OF PHYSICAL SCIENCES
DOON UNIVERSITY

PROGRAM OBJECTIVES

[1] To impart the key knowledge of chemical sciences and laboratory resources to prepare students for choosing careers 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.

[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.

DOON UNIVERSITY
2005

COURSE STRUCTURE

FIRST SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
Core	CYC-101	Inorg. Chem. I: Atomic Structure & Chemical Bonding	4	0	0	4
Core	CYL-101	Titrimetric Analysis Lab	0	0	2	2
Core	CYC-102	Phys. Chem. I: States of Matter & Ionic Equilibrium	4	0	0	4
Core	CYL-102	Physicochemical Analysis Lab	0	0	2	2
*Generic Elective	CYG-101	<i>Generic Chem.:</i> Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons	4	0	0	4
*Generic Elective	GCL-101	Inorganic and Organic Chemical Analysis Lab	0	0	2	2
**AECC	EES-110	Environmental Science	2	0	0	2
Total Credits=						20

**Generic Elective Course: The students are at liberty to choose this combination of theory and lab course or some other combination from the list of Generic Elective Courses given in Table 1. **AECC: Ability Enhancement Compulsory Course*

SECOND SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
Core	CYC-151	<i>Org. Chem. I:</i> Basics and Hydrocarbons	4	0	0	4
Core	CYL-151	Organic Compounds Purification Lab	0	0	2	2
Core	CYC-152	<i>Phys. Chem. II:</i> Chemical Thermodynamics and its Applications	4	0	0	4
Core	CYL-152	Thermochemistry Lab	0	0	2	2
*Generic Elective	CYG-151	<i>Generic Chem.:</i> Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I	4	0	0	4
*Generic Elective	GCL-151	Basic Physical and Organic Chemistry Lab	0	0	2	2
**AECC	ENG-151	English	2	0	0	2
Total Credits=						20

**Generic Elective Course: The students are at liberty to choose this combination of theory and lab course or some other combination from the list of Generic Elective Courses given in Table 1 at succeeding pages. **AECC: Ability Enhancement Compulsory Course*

THIRD SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
Core	CYC-201	Inorg. Chem. II : <i>s</i> - and <i>p</i> -Block Elements	4	0	0	4
Core	CYL-201	Quantitative Inorganic Analysis and Synthesis Lab	0	0	2	2
Core	CYC-202	Phys. Chem. III: Phase Equilibrium and Chemical Kinetics	4	0	0	4
Core	CYL-202	Chemical Kinetics Lab	0	0	2	2
Core	CYC-203	Org. Chem. II: Oxygen Containing Functional Groups	4	0	0	4
Core	CYL-203	Basic Organic Synthesis Lab	0	0	2	2
*SEC	CYS-201	Skill Enhancement Course: Fuel Chemistry	2	0	0	2
**GE	CYG-201	Generic Chem.: Chemistry of <i>s</i> - and <i>p</i> -Block Elements, States of Matter and Chemical Kinetics	4	0	0	4
**GE	GCL-201	Basic Physical and Inorganic Chemistry Lab	0	0	2	2
Total Credits=						26

*SEC (Skill Enhancement Course): The students are at liberty to choose this course or some other course from the list of SECs (Skill Enhancement Courses) given in Table 2 at succeeding pages.

**Generic Elective Course: The students are at liberty to choose this combination of theory and lab course or some other combination from the list of Generic Elective (GE) Courses given in Table 1 at succeeding pages.

FOURTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
Core	CYC-251	Inorg. Chem. III: Coordination Chemistry	4	0	0	4
Core	CYL-251	Inorganic Preparation, Separation and Gravimetric Analysis Lab	0	0	2	2
Core	CYC-252	Org. Chem. III: Heterocyclic Chemistry	4	0	0	4
Core	CYL-252	Organic Qualitative Analysis Lab	0	0	2	2
Generic	CYC-253	Phys. Chem. IV: Electrochemistry	4	0	0	4
Generic	CYL-253	Electrochemistry Lab	0	0	2	2
*SEC	CYS-255	Skill Enhancement Course: Chemistry of Cosmetics and Perfumes	2	0	0	2
**GE	CYG-252	Generic Chem.: Organometallics, Bioinorganic Chemistry, Polynuclear Hydrocarbons and UV, IR Spectroscopy	4	0	0	4
**GE	GCL-252	Inorganic and Organic Synthesis and Qualitative Analysis Lab	0	0	2	2
Total Credits =						26

*SEC (Skill Enhancement Course): The students are at liberty to choose this course or some other course from the list of SECs (Skill Enhancement Courses) given in the Table 2 at succeeding page.

**Generic Elective Course: The students are at liberty to choose this combination of theory and lab course or some other combination from the list of Generic Elective (GE) Courses given in the Table 1 at succeeding page.

FIFTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
Core	CYC-301	Org. Chem. IV: Biomolecules	4	0	0	4
Core	CYL-301	Biochemistry Lab	0	0	2	2
Core	CYC-302	Phys. Chem. V: Quantum Chemistry & Spectroscopy	4	0	0	4
Core	CYL-302	Spectroscopic Analysis Lab	0	0	2	2
*DSE	CYD-302	Discipline Specific Elective: Polymer Chemistry	04	0	0	4
*DSE	DCL-302	Polymer Chemistry Lab	02	0	2	2
*DSE	CYD-352	Discipline Specific Elective: Research Methodology for Chemistry	5	1	0	6
Total Credits =						24

*DSE: Discipline Specific Elective. This course is chosen by the students from the list of Discipline Specific Elective (DSE) Courses given in Table 3 at succeeding pages.

SIXTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
Core	CYC-351	Inorg. Chem. IV: Organometallic Chemistry	4	0	0	4
Core	CYL-351	Inorganic Synthesis and Qualitative Analysis Lab	2	0	2	2
Core	CYC-352	Org. Chem. V: Carbohydrates, Dyes, Polymers and Basics of Organic Spectroscopy	4	0	0	4
Core	CYL-352	Organic Synthesis and Qualitative Analysis Lab	2	0	2	2
*DSE	CYD-303	Discipline Specific Elective: Inorganic Materials of Industrial Importance	4	0	0	4
*DSE	DCL-303	Industrial Inorganic Materials Lab	2	0	2	2
*DSE	CYD-304	Discipline Specific Elective: Novel Inorganic Solids	4	0	0	2
*DSE	DCL-304	Materials Chemistry Lab	2	0	0	4
**DSE	DCL-310	UG Dissertation	0	0	6	6
Total Credits =						24

*DSE: Discipline Specific Elective; This course is chosen by the students from the list of Discipline Specific Elective (DSE) Courses given in Table 3 at succeeding pages.

**DSE: Discipline Specific Elective Course to be opted by the students as an alternative of either (i) combination of CYD-303 and DCL-303 or (ii) combination of CYD-304 and DCL-304

SEVENTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
Core	CYC-401	Structure and Reactivity of Organic Molecules	3	0	0	3
Core	CYC-402	Thermodynamics and Interfaces	3	0	0	3
Core	CYC-403	Solid State Chemistry	3	0	0	3
Core	CYC-404	Structure and Properties of Metal Complexes	3	0	0	3
Core	CYC-405	Instrumental Methods of Analysis-I	3	0	0	3
Core	CYL-406	Inorganic Chemistry Lab-I	0	0	2	2
Core	CYL-407	Organic Chemistry Lab-I	0	0	2	2
Core	CYL-408	Physical Chemistry Lab-I	0	0	2	2
Total Credits =						21

EIGHTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
Core	CYC- 451	<i>Pericyclic and Organic Photochemistry</i>	3	0	0	3
Core	CYC- 452	<i>Reagents and Reactions in Organic Chemistry</i>	3	0	0	3
Core	CYC- 453	<i>Kinetics and Photochemistry</i>	3	0	0	3
Core	CYC- 454	<i>Inorganic Biochemistry and Reaction Mechanism</i>	3	0	0	3
Core	CYC-455	<i>Instrumental Methods of Analysis- II</i>	3	0	0	3
Core	CYL-456	<i>Inorganic Chemistry Lab-II</i>	0	0	2	2
Core	CYL-457	<i>Organic Chemistry Lab-II</i>	0	0	2	2
Core	CYL-458	<i>Physical Chemistry Lab-II</i>	0	0	2	2
Total Credits =						21

NINTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
Core	CYL-501	Inorganic Chemistry Lab-III	0	0	2	2
Core	CYL-502	Organic Chemistry Lab-III	0	0	2	2
Core	CYL-503	Physical Chemistry Lab-III	0	0	2	2
DSE	CME-503	Green Chemistry	3	0	0	3
DSE	COE-503	Organic Structure Determination	3	0	0	3
DSE	COE-506	Organic Synthesis Lab	0	0	3	3
DSE	CPE-506	Advanced Physical Chemistry Lab	0	0	3	3
DSE	COE-507	Medicinal Chemistry	3	0	0	3
Total Credits =						21

**DSE: Discipline Specific Elective; These courses are chosen by the students from the list of Discipline Specific Elective (DSE) Courses for 9th Semester, given in Table 4.*

TENTH SEMESTER

Course Type	Course Code	Course Title	L	T	P	C
Core	CYC- 551	Thesis/Dissertation	0	0	22	11
Total Credits =						11

GUIDELINES

[1] Minimum Credit Requirements

For 03-Year B.Sc. (Hons) in Chemistry:

Course Type	Number of Courses	Credits
Core Courses	28 Course (14 Theory + 14 Lab)	14 × 4 = 56 <u>14 × 2 = 28</u> Total = 84
AECC (Ability Enhancement Compulsory Course)	2 Courses: 02 Credits each	02 × 2 = 4
SEC (Skill Enhancement Course)	2 Courses: 02 Credits each	02 × 2 = 4
Generic Elective (GE) Courses	8 Courses (04 Theory + 04 Lab)	04 × 4 = 16 <u>04 × 2 = 08</u> Total = 24
Discipline Specific Elective (DSE) Courses	08 Courses (04 Theory + 04 Lab)	04 × 4 = 16 <u>04 × 2 = 08</u> Total = 24
Total Credits		=140

Addition Two Years (4th year and 5th Year) for 05-Year Integrated M.Sc. (Chemistry)

Course Type	Number of Courses	Credits
Core	20 Courses (10 Theory + 09 Lab+ 01 Dissertation)	10×3 = 30 09×2 = 18 <u>01×11= 11</u> Total = 59
Discipline Specific Elective (DSE) Courses	5 Courses: Each of 03 Credits	05 × 3 = 15
Total Credits		= 74

It is compulsory for every student to earn a minimum of 140 credits for the award of degree of B.Sc. (Hons) in Chemistry. For the award of degree of integrated M.Sc. in Chemistry, every student will have to earn 210 credits (i.e., 140 in first 03 years + 74 credits in remaining 02-years).

[2] Generic Elective (GE) Courses

Student will have to earn 24 credits by undertaking Generic Elective courses during semesters I to IV (06 credits in semester I, 06 credits in semester II, 06 credits in semester III and 06 credits in semester IV). The students will have a liberty to choose such courses in any of the following disciplines:

❖ Physics	❖ Electronic s	❖ Statistics	❖ Computer science
❖ Electron ics	❖ Mathemat ics	❖ Operatio ns Research	❖ Commerce

Department of Chemistry will offer the following Generic Elective (GE) courses (Table 1) for the students of other disciplines:

Table 1. List of Combinations of Generic Elective Courses			
S.No.	Course Code and Title of Theory Course	S.N.	Course Code and Title of Lab Course
1(a)	<i>CYG-101: Generic Chem.: Atomic Structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons (Credits: 04)</i>	1(b)	<i>GCL-101: Inorg. and Org. Chemical Analysis Lab (Credits: 02)</i>
2(a)	<i>CYG-151: Generic Chem.: Chemical Energetics, Equilibria & Functional Group Org. Chem. I (Credits: 04)</i>	2(b)	<i>GCL-151: Basic Physical and Organic Chemistry Lab (Credits: 02)</i>
3(a)	<i>CYG-201: Generic Chem.: s- and p-Block Elements, States of Matter & Chemical Kinetics (Credits: 04)</i>	3(b)	<i>GCL-201: Basic Physical and Inorganic Chemistry Lab (Credits: 02)</i>
4(a)	<i>CYG-252: Generic Chem.: Organometallics, Bioinorganic Chemistry, Polynuclear Hydrocarbons, and UV-IR Spectroscopy (Credits: 04)</i>	4(b)	<i>GCL-252: Inorg. & Org. Synthesis and Qualitative Analysis Lab (Credits: 02)</i>
5(a)	<i>CYG-202: Generic Chem.: Chemistry of d-block elements, Quantum Chemistry and Spectroscopy (Credits: 04)</i>	5(b)	<i>GCL-202: Basic Spectroscopic Analysis Lab (Credits: 02)</i>
6(a)	<i>CYG-203: Generic Chem.: Molecules of Life (Credits: 04)</i>	6(b)	<i>GCL-203: Basic Biochemistry Lab (Credits: 02)</i>
7(a)	<i>Phase Equilibria, Electrochemistry and Qualitative Org. Analysis Lab (Credits: 04)</i>	7(b)	<i>Generic Chem.: Solutions, Phase Equilibrium, Conductance, Electrochemistry, and Functional Group Org. Chem.-I (Credits: 02)</i>

Theory and lab course will be offered in combination. Course 1(a) will be offered in combination with 1(b). Course 2(a) will be offered in combination with 2(b). Course 3(a) will be offered in combination with 3(b). Course 4(a) will be offered in combination with 4(b). Course 5(a) will be offered in combination with 5(b). Course 6(a) will be offered in combination with 6(b).

[3] Skill Enhancement Courses (SEC)

Student will have to earn 04 credits by undertaking Skill Enhancement Courses (SEC) during semesters III and Semester IV (02 credits in semester III, and 02 credits in semester IV). The students will have a liberty to choose such courses from the following list (Table 2):

Table 2. Skill Enhancement Courses (SEC) for 3rd and 4th Semesters			
S.No.	Course Code and Title	S.No.	Course Code and Title
1.	CYS-201: Fuel Chemistry (Credits: 02)	2.	CYS-251: Pesticide Chemistry (Credits: 02)
3.	CYS-255: Chemistry of Cosmetics and Perfumes (Credits: 02)	4.	IT Skills for Chemists (Credits: 02)
5.	Chemical Technology and Society (Credits: 02)	6.	Cheminformatics (Credits: 04)
7.	Business Skills for Chemists (Credits: 02)	8.	Intellectual Property Rights (IPR) (Credits: 02)
9.	Analytical Clinical Biochemistry (Credits: 02)	10.	Pharmaceutical Chemistry (Credits: 02)

[4] Discipline Specific Elective (DSE) Courses for 5th and 6th Semesters

Student will have to earn 24 credits by undertaking Discipline Specific Elective Courses during semesters V and Semester VI (12 credits in semester V, and 12 credits in semester VI). The students will have a liberty to choose such courses from the following list (Table 3):

Table 3. List of Combinations of Discipline Specific Elective (DSE) Courses For 5th and 6th Semesters			
S.No.	Course Code and Title of Theory Course	S.N.	Course Code and Title of Lab Course
1(a)	CYD-302: Discipline Specific Elective: Polymer Chemistry (Credits: 04)	1(b)	DCL-302: Polymer Chemistry Lab (Credits: 02)
2(a)	CYD-303: Discipline Specific Elective: Inorganic Materials of Industrial Importance (Credits: 04)	2(b)	DCL-303: Industrial Inorganic Materials Lab (Credits: 02)
3(a)	CYD-304: Discipline Specific Elective: Novel Inorganic Solids (Credits: 04)	3(b)	DCL-304: Materials Chemistry Lab (Credits: 02)
4(a)	CYD-305: Discipline Specific Elective: Applications of Computers in Chemistry (Credits: 04)	4(b)	DCL-305: Computational Chemistry Lab (Credits: 02)
5(a)	CYD-306: Discipline Specific Elective: Molecular Modelling and Drug Design (Credits: 04)	5(b)	DCL-306: Molecular Modelling Lab (Credits: 02)
6(a)	CYD-351: Discipline Specific Elective: Industrial Chemicals	6(b)	DCL-351: Environmental and Industrial Chemistry Lab

	and Environment (Credits: 04)		(Credits: 02)
7	CYD-352: Discipline Specific Elective: Research Methodology for Chemistry (Credits: 06)		

Theory and lab course will be offered in combination. Course 1(a) will be offered in combination with 1(b). Course 2(a) will be offered in combination with 2(b). Course 3(a) will be offered in combination with 3(b). Course 4(a) will be offered in combination with 4(b). Course 5(a) will be offered in combination with 5(b). Course 6(a) will be offered in combination with 6(b).

[5] Discipline Specific Elective (DSE) Courses for 9th Semester of Integrated M.Sc. or 3rd Semester of M.Sc.

Student will have to earn 15 credits by undertaking Discipline Specific Elective Courses during 9th semester. The students will have a liberty to choose such courses from the following list (Table 4):

Table 4. Discipline Specific Elective Courses for 9th Semester			
S.No.	<i>Course Code and Title of Inorganic Chemistry Courses</i>	S.No.	<i>Course Code and Title of Organic Chemistry Courses</i>
1.	Frontiers in Bioinorganic Chemistry (Credits: 03)	1.	Chemistry of Natural Products (Credits: 03)
2.	Inorganic Photochemistry (Credits: 03)	2.	Organic Structure Determination (Credits: 03)
3.	Supramolecular Chemistry (Credits: 03)	3.	Modern Organic Synthetic Methods (Credits: 03)
		4.	Total Organic Synthesis (IPR) (Credits: 03)
		5.	Organic Synthesis Lab (Credits: 03)
		6.	Medicinal Chemistry (Credits: 03)
S.No.	<i>Course Code and Title of Physical Chemistry Courses</i>	S.No.	<i>Course Code and Title of Multidisciplinary Courses</i>
1.	Biophysical Chemistry (Credits: 03)	1.	Environmental Pollutants and Analysis (Credits: 03)
2.	Advance Quantum Chemistry (Credits: 03)	2.	Macromolecules and Nanomaterials (Credits: 03)
3.	Solid State Chemistry and Applications (Credits: 03)	3.	Green Chemistry (Credits: 03)
4.	Advanced Surface and Colloidal Chemistry (Credits: 03)		
5.	Advanced Physical Chemistry (Credits: 03)		
6.	Advanced Physical Chemistry Lab (Credits: 03)		

[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 (06 Credits) as a Discipline Specific Elective (DSE) course at 6th Semester. At 10th semester of integrated M.Sc. (i.e., 4th semester of M.Sc.), it is compulsory for the students to carry out Dissertation (11 credits) as a core course.

The students, who undertake dissertation, participate in Research Seminars and make presentation in 6th as well as 10th semesters.



LEARNING OUTCOMES

OUTCOMES OF COURSES

IN

FIRST SEMESTER

Course Type	Course Code and Title	Course Outcome: After completing the course, the students will be able to understand:
Core	CYC-101: Inorg. Chem. I: Atomic Structure & Chemical Bonding	[CO.1] Atomic structure of elements, and various related principles and rules [CO.2] Periodic properties of elements [CO.3] Different types of chemical bonds including ionic bond, covalent bond, metallic bond and weak chemical forces [CO.4] Redox reactions and applications of electrode potential
Core	CYL-101: Titrimetric Analysis Lab	[CO.1] To prepare solutions of different molarity/normality of titrants [CO.2] To carry out titrimetric analysis [CO.3] To carry out acid-base titrations [CO.3] To perform oxidation-reduction titrimetric experiments
Core	CYC-102: Phys. Chem. I: States of Matter & Ionic Equilibrium	[CO.1] 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 [CO.2] Physical properties of liquids; vapour pressure, surface tension and cleansing action of soaps and surfactants [CO.3] 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 [CO.4] Types of electrolytes, pH, buffers and buffer action and their applications in biochemical processes, acid base volumetric titrations
Core	CYL-102: Physicochemical Analysis Lab	[CO.1] To measure viscosity and surface tension of solutions using experimental techniques [CO.2] To prepare different pH buffers [CO.3] To determine different chemical properties of acids and bases.
*Generic Elective	CYG-101: <i>Generic Chem.:</i> Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons	[CO.1] Atomic structure, quantum mechanics, Schrodinger equation and various related principles and rules [CO.2] Periodic properties of elements [CO.3] Different types of chemical bonds including ionic bond, covalent bond, VSEPR theory, hybridization, molecular orbital theory, metallic bond and weak chemical forces [CO.4] Fundamentals of organic chemistry including (i) physical effects and electronic displacements, (ii) structure, shape and reactivity of organic molecules and (iii) strengths of organic acids and bases [CO.5] Methods of preparation and chemical properties of alkanes, alkenes and alkynes [CO.6] Basic concepts of stereochemistry
*Generic Elective	GCL-101: Inorganic and Organic Chemical Analysis Lab	[CO.1] To perform volumetric analysis using acid-base titrations and oxidation-reduction titrimetric experiments [CO.2] To detect extra elements (N, S, Cl, Br, I) in organic compounds [CO.3] To separate the mixtures of organic compounds using chromatography, and also to measure the R_f value.
**AECC	EES-110: Environmental Science	[CO.1] Environmental science and its significance as well as relevance in context of human life

**OUTCOMES OF COURSES
IN
SECOND SEMESTER**

Course Type	Course Code and Title	Course Outcome <i>(After completing the course, students will be able to understand:)</i>
Core	CYC-151: <i>Org. Chem. I: Basics and Hydrocarbons</i>	[CO.1] Nomenclature, shape, and geometry of molecules [CO.2] Various electronic effects that influence acidic or basic properties of molecules. [CO.3] Electronic properties of various organic intermediates, their generation and reactivity. [CO.4] Basic concepts of nucleophilic substitution, elimination and addition reactions. [CO.5] Formation of carbon-carbon single bonds, double bonds and triple bonds. [CO.6] Conformations of alkanes and cycloalkanes, [CO.7] Basic concepts of stereochemistry and aromaticity.
Core	CYL-151: Organic Compounds Purification Lab	[CO.1] To purify the organic compounds by crystallization technique [CO.2] To determine the melting points and boiling points of unknown organic compounds [CO.3] To separate the mixture of organic compounds using chromatography
Core	CYC-152: <i>Phys. Chem. II: Chemical Thermodynamics and its Applications</i>	[CO.1] The laws of thermodynamics [CO.2] Chemical potential of an ideal mixture [CO.3] Thermodynamic equilibrium and spontaneous reactions [CO.4] Colligative properties of solutions and their applications in determination of molar masses
Core	CYL-152 : Thermochemistry Lab	[CO.1] To experimentally determine the various thermodynamic and kinetic parameters of different chemical reactions
*Generic Elective	CYG-151: <i>Generic Chem.: Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I</i>	[CO.1] Thermodynamics and its Laws, important principles and definitions of thermochemistry [CO.2] Important concepts of chemical equilibrium and ionic equilibrium [CO.3] Methods of preparation and chemical properties of aromatic hydrocarbons, alkyl halides, aryl halides, alcohols, phenols, ethers, aldehydes and ketones
*Generic Elective	GCL-151: Basic Physical and Organic Chemistry Lab	[CO.1] To determine the heat capacity of calorimeter [CO.2] To determine the enthalpies of different types of chemical reactions (such as neutralization, ionization and hydration) [CO.3] To measure the pH of different solutions using pH-meter, and to prepare buffer solutions [CO.4] To purify organic compounds by crystallization and to determine their melting and boiling points. [CO.5] To prepare some organic compounds using simple one or two-step reactions.
**AECC	ENG-151: English	[CO.1] Reading, Writing and Speaking in English

**Generic Elective Course: The students are at liberty to choose this combination of theory and lab course or some other combination from the list of Generic Elective Courses (Table 1). **AECC: Ability Enhancement Compulsory Course*

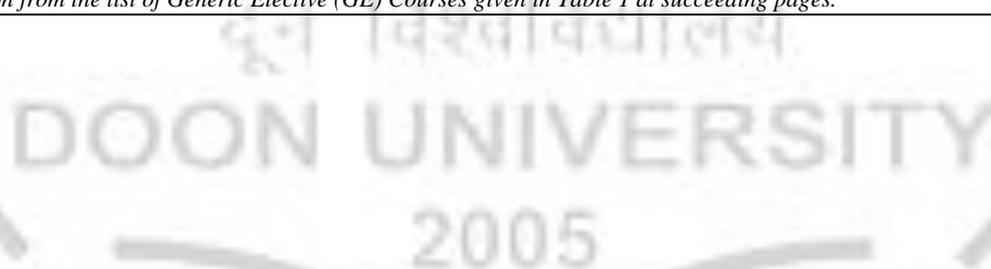
**OUTCOMES OF COURSES
IN
THIRD SEMESTER**

Course Type	Course Code and Title	Course Outcome <i>(After completing the course, students will be able to understand:)</i>
Core	CYC-201: Inorg. Chem. II : <i>s</i> - and <i>p</i> - Block Elements	[CO.1] General principles of metallurgy [CO.2] Different concepts and classification of acids and bases [CO.3] Chemistry of compounds of <i>s</i> - and <i>p</i> -block elements [CO.4] Chemistry of noble gases and their compounds such as fluorides of xenon [CO.5] Synthesis, structural aspects and applications of inorganic polymers including silicones, siloxanes, borazines, silicates and phosphazenes, and polysulphates.
Core	CYL-201: Quantitative Inorganic Analysis and Synthesis Lab	[CO.1] To carry out quantitative estimations using iodo / iodimetric titrations [CO.2] To prepare or synthesize inorganic compounds such as cuprous chloride, manganese(III) phosphate, and Potash alum or chrome alum.
Core	CYC-202: Phys. Chem. III: Phase Equilibrium and Chemical Kinetics	[CO.1] Concept of phases and phase diagram of one component system and the application of phase diagram. [CO.2] Kinetics of reactions and experimental methods of determining rates of reactions. [CO.3] Types of catalysis and mechanisms of different catalysed reactions [CO.4] Types of adsorptions and the adsorption isotherms and their applications.
Core	CYL-202: Chemical Kinetics Lab	[CO.1] Plot phase diagram of a three-component system and its application [CO.2] Get familiar with the applications of distribution law [CO.3] Apply different method to monitor and understand kinetics of chemical reactions [CO.4] Get familiar with the concept of adsorption and adsorption isotherm and their applications
Core	CYC-203: Org. Chem. II: Oxygen Containing Functional Groups	[CO.1] Methods of preparation and reactions of alkyl and aryl halides. [CO.2] Relative reactivity of alkyl, aryl, and vinyl halides towards nucleophilic substitution reactions. [CO.3] Methods of preparation and reactions of alcohols, phenols, ethers and epoxides. [CO.4] Structure, reactivity and preparation of carbonyl compounds. [CO.5] Preparation and reactions of carboxylic compounds, acid chlorides, anhydrides, esters and amides.
Core	CYL-203: Basic Organic Synthesis Lab	[CO.1] To identify the functional group (such as alcohols, phenols, carbonyl and carboxylic acid group) in organic compound by performing chemical tests [CO.2] To prepare and synthesize organic compounds by performing reactions (such as acetylation, benzoylation, oxidation of ethanol/ isopropanol

		(iodoform reaction), bromination, nitration, selective reduction, hydrolysis, aldol condensation and benzil-benzilic acid rearrangement [CO.3] To experimentally generate the nucleophile from substituted thiophenol(s) and use it in nucleophilic substitution reaction
*SEC	CYS–201: Skill Enhancement Course: Fuel Chemistry	[CO.1] Renewable and non-renewable sources of energy, different types of fuels and their calorific values [CO.2] Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. [CO.3] Coal gas, producer gas and water gas—composition and uses. [CO.4] Petroleum, petrochemical industry, different types of petroleum products and their applications. [CO.5] Lubricants and their classification, properties of lubricants (viscosity index, cloud point, pore point) and their determination.
**GE	CYG–201: Generic Chem.: Chemistry of <i>s</i> - and <i>p</i> -Block Elements, States of Matter and Chemical Kinetics	[CO.1] General principles of metallurgy, and methods of purification of metals [CO.2] Chemistry of <i>s</i> and <i>p</i> block elements and their compounds including hydrides of nitrogen, oxoacids of P, S and Cl and halides and oxohalides [CO.3] Kinetic theory of gases [CO.4] Surface tension and viscosity of liquids [CO.5] Chemical kinetics including the concepts of the reaction rates and the theories of reaction rates
**GE	GCL–201: Basic Physical and Inorganic Chemistry Lab	[CO.1] To perform semi-micro qualitative analysis for identifying cations and anions [CO.2] To measure the surface tension and viscosity of liquids [CO.3] To study the kinetics of the chemical reactions

*SEC (Skill Enhancement Course): The students are at liberty to choose this course or some other course from the list of SECs (Skill Enhancement Courses) given in Table 2 at succeeding pages.

**Generic Elective Course: The students are at liberty to choose this combination of theory and lab course or some other combination from the list of Generic Elective (GE) Courses given in Table 1 at succeeding pages.



OUTCOMES OF COURSES

IN FOURTH SEMESTER

Course Type	Course Code and Title	After completing the course, students will be able to understand:
Core	CYC-251: <i>Inorg. Chem. III:</i> Coordination Chemistry	[CO.1] IUPAC nomenclature, isomerism, stereochemistry and various theories of coordination compounds. [CO.2] 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] Properties of Lanthanoids and Actinoids [CO.4] Chemistry of metal ions present in biological systems
Core	CYL-251: Inorganic Preparation, Separation and Gravimetric Analysis Lab	[CO.1] To carry out gravimetric analysis for quantitative estimation of different metals such as nickel, copper, iron and aluminium. [CO.2] To prepare and synthesize inorganic coordination compounds such as tetraamminecopper (II) sulphate, $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$, <i>cis</i> and <i>trans</i> Potassium dioxalatodiaquachromate (III), tetraamminecarbonatocobalt (III) ion and potassium tris(oxalate)ferrate(III) [CO.3] To learn the principles involved in chromatographic separations of metal ions and to separate the metal ions using paper chromatographic technique.
Core	CYC-252: <i>Org. Chem. III:</i> Heterocyclic Chemistry	[CO.1] Various organic compounds having nitrogen containing functional groups. [CO.2] Reactivity and basicity of alkyl and aryl amines. The difference between nucleophilic and basic amines. [CO.3] Structure and reactions of polynuclear hydrocarbons such as naphthalene, phenanthrene and anthracene. [CO.4] Classification, nomenclature, and named synthesis of various heterocyclic compounds. [CO.5] Natural occurrence, classification, synthesis and medicinal properties of alkaloids and terpenes.
Core	CYL-252: Organic Qualitative Analysis Lab	[CO.1] To detect extra elements in organic compounds [CO.2] To identify the functional groups (such as nitro, amine and amide) in the organic compounds by performing the chemical tests. [CO.3] To carry out the qualitative analysis of unknown organic compounds [CO.4] To carry out the chemical reactions between amines and carbonyl compounds
Core	CYC-253: <i>Phys. Chem. IV:</i> Electrochemistry	[CO.1] Concept of conductivity in electrolytes and dilute solutions [CO.2] Ionic velocities and ion mobility and methods of their determination [CO.3] Different thermodynamic parameters for chemical reactions, comprehend the redox processes in electrochemical systems [CO.4] Applications of conductance measurement [CO.5] Laws of electrochemistry and their applications [CO.6] Chemical cells and applications of EMF measurements

Core	CYL-253: Electrochemistry Lab	[CO.1] To measure the conductance of the electrolytes using electroanalytical methods namely conductometry and potentiometry methods [CO.2] To handle the electroanalytical techniques and explore their applications
*SEC	CYS-255: <i>Skill Enhancement Course:</i> Chemistry of Cosmetics and Perfumes	[CO.1] 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] 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 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.
**GE	CYG-252: <i>Generic Chem.:</i> Organometallics, Bioinorganic Chemistry, Polynuclear Hydrocarbons and UV, IR Spectroscopy	[CO.1] Chemistry of transition metals of 3d series [CO.2] Organometallic compounds and their classification, structural aspects of methyl lithium, Zeiss salt and ferrocene [CO.3] Preparation, structure, properties and bonding of mononuclear and polynuclear metal carbonyls of 3d series [CO.4] Bioinorganic chemistry, and metal ions in biological systems [CO.5] Fundamentals of UV-Vis and IR spectroscopy [CO.6] Use of UV-Vis and IR spectra in qualitative analysis and structural elucidation of organic compounds [CO.7] Methods of preparation and chemical properties of active methylene compounds and polynuclear and heteronuclear aromatic compounds
**GE	GCL-252: Inorganic and Organic Synthesis and Qualitative Analysis Lab	[CO.1] To separation of mixtures of inorganic ions using paper chromatographic techniques and measure the R_f value [CO.2] To prepare and synthesize inorganic coordination compounds [such as tetraamminecarbonatocobalt (III) nitrate, tetraamminecopper (II) sulphate and potassium trioxalatoferrate (III) trihydrate], and measure their conductivity. [CO.3] To carry out qualitative analysis of simple monofunctional organic compounds having only one functional group [CO.4] To prepare and synthesize the simple organic compounds having only one functional group (such as -COOH, phenolic, aldehydic, ketonic, amide, nitro, amines)

*SEC (*Skill Enhancement Course*): The students are at liberty to choose this course or some other course from the list of SECs (*Skill Enhancement Courses*).

**Generic Elective Course: The students are at liberty to choose this combination of theory and lab course or some other combination from the list of *Generic Elective (GE) Courses*.

**OUTCOMES OF COURSES
IN
FIFTH SEMESTER**

Course Type	Course Code and Title	Course Outcome: <i>After completing the course, students will be able to understand:</i>
Core	CYC-301: Org. Chem. IV: Biomolecules	[CO.1] Structures of genetic material DNA and RNA, the constituting nucleobases, nucleotides and their synthesis. [CO.2] Structure and classification of amino acids. Synthesis of peptides and methods for analysing amino acids sequences. [CO.3] Classification and mechanism of enzymes. Factors influencing enzyme's activity, enzyme inhibitors and their importance. [CO.4] Classification and importance of fats, oil and lipids. [CO.5] Food metabolism, process of conversion of food into energy and use of energy in the synthesis of complex biomolecules. [CO.6] Structure, synthesis and medicinal importance of some pharmaceutical compounds.
Core	CYL-301: Biochemistry Lab	[CO.1] 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.2] To carry out the estimation of proteins using Lowry's method. [CO.3] To study the action of salivary amylase on starch, and the effect of temperature on such action [CO.4] To determine the saponification value of an oil or a fat. [CO.5] To determine the iodine number of an oil/ fat. [CO.6] To isolate and characterize the DNA from onion/cauliflower/peas.
Core	CYC-302: Phys. Chem. V: Quantum Chemistry & Spectroscopy	[CO.1] Schrodinger equation for a particle in a box and quantum chemical description. [CO.2] Electronic and Hamiltonian operators for molecules. [CO.3] Quantum chemical description of angular momentum and term symbols for a one and many-electron systems. [CO.4] LCAO-MO treatment for H ₂ molecule, Born-Oppenheimer approximation. [CO.5] Interaction of electromagnetic radiation with molecules and various types of spectra and their principles. [CO.6] Laws of photochemistry and concept of photochemical reactions and their role in biochemical processes.
Core	CYL-302: Spectroscopic Analysis Lab	[CO.1] Record and interpret UV-Vis Spectra of common chemicals [CO.2] Apply the electronic spectroscopy in studying the kinetics of the reactions
*DSE	CYD-302: <i>Discipline Specific Elective:</i> Polymer Chemistry	CO.1] History, classification and nomenclature of polymers. [CO.2] Molecular forces and chemical bonding in polymers, and texture of polymers. [CO.3] Criteria for synthetic polymer formation and classification of polymerization processes, Relationships

		<p>between functionality</p> <p>[CO.4] Mechanism and kinetics of step growth, radical chain growth, ionic chain and coordination polymerizations.</p> <p>[CO.5] Mechanism and kinetics of copolymerization and polymerization techniques.</p> <p>[CO.6] Crystallization and crystallinity of polymers</p> <p>[CO.7] Structure property relationships in polymers</p> <p>[CO.8] Determination of molecular weights and glass transition temperature of polymers</p> <p>[CO.9] Physical, thermal, flow & mechanical properties of polymers</p>
*DSE	DCL-302: Polymer Chemistry Lab	<p>[CO.1] To carry out various polymerization reactions such as free radical solution polymerization, redox polymerization, and precipitation polymerization, and microscale emulsion polymerization</p> <p>[CO.2] To prepare and synthesize simple polymers such as nylon 66/6, polyester, urea-formaldehyde resin, novalac resin/resold resin and poly(methylacrylate).</p> <p>[CO.3] To characterize the polymers by determining the molecular weight using different methods such as viscometry, and end group analysis.</p> <p>[CO.4] To test the mechanical properties of polymers.</p> <p>[CO.5] To analyse the polymers using instrumental techniques</p>
*DSE	CYD-352: <i>Discipline Specific Elective: Research Methodology for Chemistry</i>	<p>O.1] Printed sources of information for literature survey, digital sources of information for literature survey, and information technology and library resources</p> <p>[CO.2] Methods of scientific research and writing scientific papers, writing ethics, and avoiding plagiarism.</p> <p>[CO.3] 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.</p> <p>[CO.4] Data analysis, the investigative approach, and analysis and presentation of data</p> <p>[CO.5] Basic fundamentals of electronic circuits and their components used in circuits of common instruments like spectrophotometers.</p>

*DSE: *Discipline Specific Elective. This course is chosen by the students from the list of Discipline Specific Elective (DSE) Courses.*

OUTCOMES OF COURSES

IN SIXTH SEMESTER

Course Type	Course Code and Title	Course Outcome: <i>After completing the course, students will be able to understand:</i>
Core	CYC-351: <i>Inorg. Chem. IV:</i> Organometallic Chemistry	[CO.1] Basic principles involved in analysis of cations and anions (including solubility products and common ion effect). [CO.2] Principles involved in separation of cations [CO.3] Interfering anions (fluoride, borate, etc) [CO.3] Organometallic compounds, their definition, their classification, 18 electron rule, EAN rule, hapticity of ligands [CO.4] Organometallic compounds (<i>viz.</i> Zeise salt, metal alkyls and ferrocene) and their properties [CO.5] Reaction kinetics and mechanism of substitution reactions in octahedral complexes and square planar complexes [CO.6] Applications of organometallic compounds as catalysts in different industrial processes
Core	CYL-351: Inorganic Synthesis and Qualitative Analysis Lab	[CO.1] To perform qualitative semimicro-analysis of mixtures containing inorganic anions and cations. [CO.2] To use spectrophotometric method for the measurement of 10 Dq. [CO.3] To verify the spectrochemical series. [CO.4] To carry out controlled synthesis of two copper oxalate hydrate complexes on the basis of kinetic versus thermodynamic factors. [CO.5] To prepare and synthesize acetylacetonato complexes of copper or iron and find out their λ_{max} value experimentally. [CO.6] To prepare and synthesize the ammine complexes of metal (such as nickel) and perform its ligand exchange reactions by substitution method.
Core	CYC-352: <i>Org. Chem. V:</i> Carbohydrates, Dyes, Polymers and Basics of Organic Spectroscopy	[CO.1] Fundamentals of UV-Vis, IR and NMR spectroscopy. [CO.2] Use of UV-Vis, IR and NMR spectra in qualitative analysis and structural elucidation of organic compounds [CO.3] Nomenclature, classification and synthesis of carbohydrates. [CO.4] How to draw structures of carbohydrates in different projections and their inter-conversion. [CO.5] Classification, colour, constituents and synthesis of different dyes. [CO.5] Polymers, their classification, methods of their preparation and their uses.
Core	CYL-352: Organic Synthesis and Qualitative Analysis Lab	[CO.1] To extract organic compound(s) (such as caffeine) from natural sources (such as tea leaves). [CO.2] To prepare and synthesize simple polymers and dyes (such as sodium polyacrylate, urea formaldehyde, and methyl orange) [CO.3] To analyse the carbohydrates including aldoses and ketoses, reducing and non-reducing sugars. [CO.4] To perform qualitative analysis of organic

		<p>compounds containing one or two functional groups.</p> <p>[CO.5] To apply IR spectroscopic and NMR spectroscopic techniques for identification of simple organic compounds with the help of their spectra.</p>
*DSE	<p>CYD-303: Discipline Specific Elective: Inorganic Materials of Industrial Importance</p>	<p>[CO.1] Inorganic materials (such as glass, ceramics and cements) of silicate industries</p> <p>[CO.2] Types and manufacturing of common fertilizers</p> <p>[CO.3] Surface coating, its classification, paints and pigments, fillers, thinners, enamels, emulsifying agents.</p> <p>[CO.4] Dyes, wax polishing, water and oil paints, additives, metallic coatings (electrolytic and electroless), metal spraying and anodizing.</p> <p>[CO.5] Batteries, their components and working of different types of batteries</p> <p>[CO.6] Alloys and their classification of alloys, types of alloys, specific properties of elements in alloys, manufacturing of steel</p> <p>[CO.7] Principles and properties of catalysts, homogenous catalysis, heterogenous catalysis, and their industrial applications</p> <p>[CO.8] Chemical explosives, preparation and explosive properties of lead azide, PETN, cyclonite (RDX).</p> <p>[CO.9] Rocket propellants</p>
*DSE	<p>DCL-303: Industrial Inorganic Materials Lab</p>	<p>[CO.1] To analyse the inorganic materials or compounds (such as fertilizers, cement, alloys, pigments) of industrial importance</p> <p>[CO.2] To determine (i) free acidity in ammonium sulphate fertilizer, (ii) composition of dolomite with the help of complexometric titration.</p> <p>[CO.3] To estimate (i) calcium in calcium ammonium nitrate fertilizer, (ii) phosphoric acid in superphosphate fertilizer, (iii)</p> <p>[CO.4] To analyse cement and alloys or synthetic samples.</p> <p>[CO.5] To prepare the pigment (zinc oxide).</p>
*DSE	<p>CYD-304: Discipline Specific Elective: Novel Inorganic Solids</p>	<p>[CO.1] Various methods of synthesis and modification of inorganic solids</p> <p>[CO.2] Inorganic solids (solid electrolytes, mixed inorganic pigments, molecular material, fullerides, molecular magnets, inorganic liquid crystals) of technological importance</p> <p>[CO.3] Nanomaterials, their classification, Au and Ag nanostructures, carbon nanotubes and inorganic nanowires, bio-inorganic nanomaterials, DNA and nanomaterials, and bionano composites.</p> <p>[CO.4] Composition, mechanical and fabricating characteristics and applications of various types of engineering materials (such as cast irons, plain carbon and alloy steels, copper, aluminum and their alloys like duralumin, brasses and bronzes cutting tool materials, super alloys thermoplastics, thermosets and composite materials.</p> <p>[CO.5] Composite materials, environmental effects on composites and applications</p> <p>[CO.6] Conducting polymers, their applications, ion exchange resins and their applications, ceramic and</p>

		refractory materials and their applications.
*DSE	DCL-304: Materials Chemistry Lab	[CO.1] Different methods used for the determination of novel inorganic solids. [CO.2] To apply cation exchange method [CO.3] To determine total difference of solids. [CO.4] To carry out the synthesis of (i) hydrogel by co-precipitation method (ii) silver and gold metal nanoparticles.
**DSE	DCL-310: UG Dissertation	To carry out research (experimental or computational work) and write the scientific report and article.

*DSE: Discipline Specific Elective courses. These are non-semester specific courses. This course is chosen by the students from the list of Discipline Specific Elective (DSE) Courses.

**DSE: Discipline Specific Elective Course. UG Dissertation is a semester-specific course. It is offered only in the 6th semester. The students may opt it as an alternative of either (i) combination of CYD-303 and DCL-303 or (ii) combination of CYD-304 and DCL-304.



**OUTCOMES
OF
GENERIC ELECTIVE (GE) COURSES**

(To be offered to the students during Semester 1-4)

Course Outcomes		
S.No.	Course Code and Title	<i>After completing the course, students will be able to understand:</i>
1(a)	<i>CYG-101: Generic Chem.: Atomic Structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons (Credits: 04)</i>	[CO.1] Atomic structure, quantum mechanics, Schrodinger equation and various related principles and rules [CO.2] Periodic properties of elements [CO.3] Different types of chemical bonds including ionic bond, covalent bond, VSEPR theory, hybridization, molecular orbital theory, metallic bond and weak chemical forces [CO.4] Fundamentals of organic chemistry including (i) physical effects and electronic displacements, (ii) structure, shape and reactivity of organic molecules and (iii) strengths of organic acids and bases [CO.5] Methods of preparation and chemical properties of alkanes, alkenes and alkynes [CO.6] Basic concepts of stereochemistry
1(b)	<i>GCL-101: Inorg. and Org. Chemical Analysis Lab (Credits: 02)</i>	[CO.1] To perform volumetric analysis using acid-base titrations and oxidation-reduction titrimetric experiments [CO.2] To detect extra elements (N, S, Cl, Br, I) in organic compounds [CO.3] To separate the mixtures of organic compounds using chromatography, and also to measure the R_f value.
2(a)	<i>CYG-151: Generic Chem.: Chemical Energetics, Equilibria & Functional Group Org. Chem. I (Credits: 04)</i>	[CO.1] Thermodynamics and its Laws, important principles and definitions of thermochemistry [CO.2] Important concepts of chemical equilibrium and ionic equilibrium [CO.3] Methods of preparation and chemical properties of aromatic hydrocarbons, alkyl halides, aryl halides, alcohols, phenols, ethers, aldehydes and ketones
2(b)	<i>GCL-151: Basic Physical and Organic Chemistry Lab (Credits: 02)</i>	[CO.1] To determine the heat capacity of calorimeter [CO.2] To determine the enthalpies of different types of chemical reactions (such as neutralization, ionization and hydration) [CO.3] To measure the pH of different solutions using pH-meter, and to prepare buffer solutions [CO.4] To purify organic compounds by crystallization and to determine their melting and boiling points. [CO.5] To prepare some organic compounds using simple one or two-step reactions.
3(a)	<i>CYG-201: Generic Chem.: s- and p-Block Elements, States of Matter & Chemical Kinetics (Credits: 04)</i>	[CO.1] General principles of metallurgy, and methods of purification of metals [CO.2] 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.3] Kinetic theory of gases

		[Co.4] Surface tension and viscosity of liquids [CO.5] Chemical kinetics including the concepts of the reaction rates and the theories of reaction rates
3(b)	GCL-201: Basic Physical and Inorganic Chemistry Lab (Credits: 02)	[CO.1] To perform semi-micro qualitative analysis for identifying cations and anions [CO.2] To measure the surface tension and viscosity of liquids [CO.3] To study the kinetics of the chemical reactions
4(a)	CYG-252: Generic Chem.: Organometallics, Bioinorganic Chemistry, Polynuclear Hydrocarbons, and UV-IR Spectroscopy (Credits: 04)	[CO.1] Chemistry of transition metals of 3d series [CO.2] Definition and classification of organometallic compounds, structural aspects of methyl lithium, Zeiss salt and ferrocene [CO.3] Preparation, structure, properties and bonding of mononuclear and polynuclear metal carbonyls of 3d series [CO.4] Bioinorganic chemistry, and metal ions in biological systems [CO.5] Fundamentals of UV-Vis and IR spectroscopy [CO.6] Use of UV-Vis and IR spectra in qualitative analysis and structural elucidation of organic compounds [CO.7] Methods of preparation and chemical properties of active methylene compounds and polynuclear and heteronuclear aromatic compounds
4(b)	GCL-252: Inorg. & Org. Synthesis and Qualitative Analysis Lab (Credits: 02)	[CO.1] To separation of mixtures of inorganic ions using paper chromatographic techniques and measure the <i>R_f</i> value [CO.2] To prepare and synthesize inorganic coordination compounds [such as tetraamminecarbonatocobalt (III) nitrate, tetraamminecopper (II) sulphate and potassium trioxalatoferrate (III) trihydrate], and measure their conductivity. [CO.3] To carry out qualitative analysis of simple monofunctional organic compounds having only one functional group [CO.4] To prepare and synthesize the simple organic compounds having only one functional group (such as -COOH, phenolic, aldehydic, ketonic, amide, nitro, amines)
5(a)	CYG-202: Generic Chem.: Chemistry of <i>d</i> -block elements, Quantum Chemistry and Spectroscopy (Credits: 04)	[CO.1] Properties of transition elements of 3d series as well as lanthanoids and actinoids [CO.2] Coordination chemistry with examples of the metals e.g., chromium, iron, cobalt, nickel and copper [CO.3] Crystal field theory and Jahn Teller distortion [CO.4] Postulates of quantum mechanics and quantum mechanical operators [CO.5] Electronic spectroscopy and photochemistry
5(b)	GCL-202: Basic Spectroscopic Analysis Lab (Credits: 02)	[CO.1] To carry out quantitative analysis or estimation of ions of various metals (such as nickel, aluminium, magnesium, zinc, sodium or potassium) using different techniques including gravimetric

		analysis, complexometric titrations, UV-Visible spectroscopy and flame photometry [CO.2] To record UV spectra of acetone, acetaldehyde, 2-propanol or acetic acid in water [CO.3] To calculate the energies of the electronic transitions in KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ with help of values of λ_{max} in absorbance spectra. [CO.4] To study the pH-dependence of the UV-Vis spectrum of $\text{K}_2\text{Cr}_2\text{O}_7$.
6(a)	CYG-203: Generic Chem.: Molecules of Life (Credits: 04)	[CO.1] Classification, properties and structure of carbohydrates [CO.2] Amino acids, peptides and proteins [CO.3] Enzymes and their correlation with drug design [CO.4] Nucleic acids, genetic code, biological roles of DNA and RNA, replication, transcription and translation [CO.5] Lipids, their classification and biological importance [CO.6] Basic concepts of energy in biosystems
6(b)	GCL-203: Basic Biochemistry Lab (Credits: 02)	[CO.1] To carry out separation of amino acids using paper chromatography [CO-2] 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.3] To carry out the estimation of proteins using Lowry's method. [CO.4] To study the action of salivary amylase on starch, and the effect of temperature on such action [CO.5] To determine the saponification value of an oil or a fat. [CO.6] To determine the iodine number of an oil/ fat. [CO.7] To isolate and characterize the DNA from onion/cauliflower/peas.
7(a)	Generic Chem.: Solutions, Phase Equilibrium, Conductance, Electrochemistry, and Functional Group Org. Chem.-II (Credits: 04)	[CO.1] The concepts of solutions, phase equilibrium, conductance and electrochemistry [CO.2] Methods of preparation and chemical properties of carboxylic acids, derivatives of carboxylic acids, amines and diazonium salts [CO.3] Methods of preparation and properties of amino acids, peptides and proteins [CO.4] Carbohydrates, their classification and properties
7(b)	Phase Equilibria, Electrochemistry and Qualitative Org. Analysis Lab (Credits: 02)	[CO.1] To construct the phase diagram of a binary system (simple eutectic) using cooling curves. [CO.2] 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 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 perform the experiments in the laboratory to carry out conductometric titrations. [CO.5] To carry out the experiments for the estimation of glycine by Sorenson's formalin method, and also to study the titration curve of

		<p>glycine.</p> <p>[CO.6] To carry out the estimation of proteins using Lowry's method.</p> <p>[CO.7] To study the action of salivary amylase on starch, and the effect of temperature on such action</p> <p>[CO.8] To determine the saponification value of an oil or a fat.</p> <p>[CO.9] To determine the iodine number of an oil/ fat.</p> <p>[CO.10] To isolate and characterize the DNA from onion/ cauliflower/</p>
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Theory and lab course will be offered in combination. Course 1(a) will be offered in combination with 1(b). Course 2(a) will be offered in combination with 2(b). Course 3(a) will be offered in combination with 3(b). Course 4(a) will be offered in combination with 4(b). Course 5(a) will be offered in combination with 5(b). Course 6(a) will be offered in combination with 6(b).



**OUTCOMES
OF
SKILL ENHANCEMENT COURSES (SEC)**

Course Outcomes		
S.No.	<i>Course Code and Title</i>	<i>After completing the course, students will be able to understand:</i>
1.	CYS-201: Fuel Chemistry (Credits: 02)	<p>[CO.1] Renewable and non-renewable sources of energy, different types of fuels and their calorific values</p> <p>[CO.2] Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal.</p> <p>[CO.3] Coal gas, producer gas and water gas—composition and uses.</p> <p>[CO.4] Petroleum, petrochemical industry, different types of petroleum products and their applications.</p> <p>[CO.5] Lubricants and their classification, properties of lubricants (viscosity index, cloud point, pour point) and their determination.</p>
2.	CYS-251: Pesticide Chemistry (Credits: 02)	<p>[CO.1] Pesticides (natural and synthetic) and their benefits and adverse effects.</p> <p>[CO.2] Changing concepts of pesticides and structure activity relationship.</p> <p>[CO.3] Synthesis and technical manufacturing of (i) DDT i.e., gamma-xene (ii) malathion, carbofuran and carbaryl, chloranil, alachlor and butachlor.</p> <p>[CO.4] To perform experiments in the laboratory to calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.</p> <p>[CO.5] To perform experiments in the laboratory to synthesize and prepare simple organophosphates, phosphonates and thiophosphates</p>
3.	CYS-255: Chemistry of Cosmetics and Perfumes (Credits: 02)	<p>[CO.1] 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.</p> <p>[CO.2] Essential oils (such as eugenol, geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, jasmone, civetone, muscone and their importance in cosmetic industries.</p> <p>[CO.3] 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.</p>

4.	IT Skills for Chemists (Credits: 02)	[CO.1] 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] Computer programming [CO.3] Introductory writing activities using word processor and structure drawing (ChemSketch) software. [CO.4] Handling data using spreadsheet software (Excel), plotting graphs using a spreadsheet, spectral data etc. [CO.5] Statistical analysis
5.	Chemical Technology and Society (Credits: 02)	[CO.1] Chemical technology including distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. [CO.2] Scope of different types of equipments including reactors, distillation columns, extruders, pumps, mills, emulgators. [CO.3] Scaling up operations in chemical industry and clean technology [CO.4] Societal and technological issues from a chemical perspective
6.	Cheminformatics (Credits: 04)	[CO.1] History, evolution, use, and prospects of chemoinformatics. [CO.2] Molecular modelling and structure elucidation. [CO.3] Representation of molecules and chemical reactions [CO.4] Different applications of cheminformatics
7.	Business Skills for Chemists (Credits: 02)	[CO.1] Basics key business concepts including business plans, market need, project management and routes to market. [CO.2] Current challenges and opportunities for the chemistry in industries. [CO.3] Role of chemistry in India and global economies. [CO.4] Financial aspects of business with case studies [CO.5] Concept of intellectual property including patents
8.	Intellectual Property Rights (IPR) (Credits: 02)	[CO.1] Introduction, historical perspective, types and importance of intellectual property. [CO.2] Difference between copyrights and patents. [CO.3] Trademarks and their types including collective marks, certification marks, service marks, trade names, etc. [CO.4] Patents [CO.5] Geographical Indications [CO.6] Industrial designs

		<p>[CO.7] Trade secrets</p> <p>[CO.8] Different international agreements including (a) world trade organization (WTO) (b) Paris Convention</p> <p>[CO.9] WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity</p> <p>[CO.10] IP Infringement issue and enforcement</p>
9.	<p>Analytical Clinical Biochemistry</p> <p><i>(Credits: 02)</i></p>	<p>[CO.1] Structures, properties and functions of carbohydrates, proteins, enzymes, lipoproteins and DNA</p> <p>[CO.2] Blood and urine analysis and to use the data and results as a diagnostic approach for correlating with biochemistry of disease</p> <p>[CO.3] To perform qualitative and quantitative analysis in the laboratory to identify and estimate (i) carbohydrates and (ii) lipids – qualitative.</p> <p>[CO.4] To determine (i) iodine number of oil, (ii) saponification number of oil, (iii) cholesterol using Liebermann- Burchard reaction</p> <p>[CO.5] To carry out qualitative analysis of proteins</p> <p>[CO.6] To isolate protein, and determine it using the Biuret reaction</p> <p>[CO.7] To determine the nucleic acids</p>
10.	<p>Pharmaceutical Chemistry</p> <p><i>(Credits: 02)</i></p>	<p>[CO.1] Drug discovery, design and development.</p> <p>[CO.2] Synthesis of 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.</p> <p>[CO.3] Difference between aerobic and anaerobic fermentation.</p> <p>[CO.4] 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.</p> <p>[CO.5] To prepare and synthesize aspirin in laboratory and analyse it</p> <p>[CO.6] To prepare and synthesize magnesium bisilicate (antacid) in the laboratory</p>

**OUTCOMES
OF
DISCIPLINE SPECIFIC ELECTIVE COURSES
IN
5th and/or 6th Semesters**

Course Outcomes		
S.No.	<i>Course Code and Title</i>	<i>After completing the course, students will be able to understand:</i>
1(a)	CYD-302: Discipline Specific Elective: Polymer Chemistry (Credits: 04)	<p>[CO.1] History, classification and nomenclature of polymers.</p> <p>[CO.2] Molecular forces and chemical bonding in polymers, and texture of polymers.</p> <p>[CO.3] Criteria for synthetic polymer formation and classification of polymerization processes, Relationships between functionality</p> <p>[CO.4] Mechanism and kinetics of step growth, radical chain growth, ionic chain and coordination polymerizations.</p> <p>[CO.5] Mechanism and kinetics of copolymerization and polymerization techniques.</p> <p>[CO.6] Crystallization and crystallinity of polymers</p> <p>[CO.7] Structure property relationships in polymers</p> <p>[CO.8] Determination of molecular weights and glass transition temperature of polymers</p> <p>[CO.9] Physical, thermal, flow & mechanical properties of polymers</p>
1(b)	DCL-302: Polymer Chemistry Lab (Credits: 02)	<p>[CO.1] To carry out various polymerization reactions such as free radical solution polymerization, redox polymerization, and precipitation polymerization, and microscale emulsion polymerization</p> <p>[CO.2] To prepare and synthesize simple polymers such as nylon 66/6, polyester, urea-formaldehyde resin, novalac resin/resold resin and poly(methylacrylate).</p> <p>[CO.3] To characterize the polymers by determining the molecular weight using different methods such as viscometry, and end group analysis.</p> <p>[CO.4] To test the mechanical properties of polymers.</p> <p>[CO.5] To analyse the polymers using instrumental techniques</p>
2(a)	CYD-303: Discipline Specific Elective: Inorganic Materials of Industrial Importance (Credits: 04)	<p>[CO.1] Inorganic materials (such as glass, ceramics and cements) of silicate industries</p> <p>[CO.2] Types and manufacturing of common fertilizers</p> <p>[CO.3] Surface coating, its classification, paints and pigments, fillers, thinners,</p>

		<p>enamels, emulsifying agents.</p> <p>[CO.4] Dyes, wax polishing, water and oil paints, additives, metallic coatings (electrolytic and electroless), metal spraying and anodizing.</p> <p>[CO.5] Batteries, their components and working of different types of batteries</p> <p>[CO.6] Alloys and their classification of alloys, types of alloys, specific properties of elements in alloys, manufacturing of steel</p> <p>[CO.7] Principles and properties of catalysts, homogenous catalysis, heterogenous catalysis, and their industrial applications</p> <p>[CO.8] Chemical explosives, preparation and explosive properties of lead azide, PETN, cyclonite (RDX).</p> <p>[CO.9] Rocket propellants.</p>
2(b)	<p>DCL-303: Industrial Inorganic Materials Lab (Credits: 02)</p>	<p>[CO.1] To analyse the inorganic materials or compounds (such as fertilizers, cement, alloys, pigments) of industrial importance</p> <p>[CO.2] To determine (i) free acidity in ammonium sulphate fertilizer, (ii) composition of dolomite with the help of complexometric titration.</p> <p>[CO.3] To estimate (i) calcium in calcium ammonium nitrate fertilizer, (ii) phosphoric acid in superphosphate fertilizer, (iii)</p> <p>[CO.4] To analyse cement and alloys or synthetic samples.</p> <p>[CO.5] To prepare the pigment (zinc oxide).</p>
3(a)	<p>CYD-304: Discipline Specific Elective: Novel Inorganic Solids (Credits: 04)</p>	<p>[CO.1] Various methods of synthesis and modification of inorganic solids</p> <p>[CO.2] Inorganic solids (solid electrolytes, mixed inorganic pigments, molecular material, fullerides, molecular magnets, inorganic liquid crystals) of technological importance</p> <p>[CO.3] Nanomaterials, their classification, Au and Ag nanostructures, carbon nanotubes and inorganic nanowires, bio-inorganic nanomaterials, DNA and nanomaterials, and bionano composites.</p> <p>[CO.4] Composition, mechanical and fabricating characteristics and applications of various types of engineering materials (such as cast irons, plain carbon and alloy steels, copper, aluminum and their alloys like duralumin, brasses and bronzes cutting tool materials, super alloys thermoplastics, thermosets and composite materials.</p> <p>[CO.5] Composite materials, environmental effects on composites and applications</p>

		[CO.6] Conducting polymers, their applications, ion exchange resins and their applications, ceramic and refractory materials and their applications.
3(b)	DCL-304: Materials Chemistry Lab (Credits: 02)	[CO.1] Different methods used for the determination of novel inorganic solids. [CO.2] To apply cation exchange method [CO.3] To determine total difference of solids. [CO.4] To carry out the synthesis of (i) hydrogel by co-precipitation method (ii) silver and gold metal nanoparticles.
4(a)	CYD-305: Discipline Specific Elective: Applications of Computers in Chemistry (Credits: 04)	[CO.1] Basics of computer applications such as constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. [CO.2] Elements of the basic language. [CO.3] Basic keywords and commands. [CO.4] Logical and relative operators, strings and graphics. [CO.5] Compiled versus interpreted languages, debugging. [CO.6] Simple programs, matrix addition and multiplication. [CO.7] statistical analysis. [CO.8] Numerical methods including roots of equations, differential calculus, integral calculus, simultaneous equations, interpolation, extrapolation and curve fitting, [CO.9] Conceptual background of molecular modelling
4(b)	DCL-305: Computational Chemistry Lab (Credits: 02)	[CO.1] Roots of equations: (e.g., volume of van der Waals gas and comparison with ideal gas, pH of a weak acid). [CO.2] Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations). [CO.3] Numerical integration (e.g. entropy/enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values. [CO.4] Matrix operations and their application of Gauss-Siedel method in colourimetry. [CO.5] To use molecular visualization software, and carry out simple exercise.
5(a)	CYD-306: Discipline Specific Elective: Molecular Modelling and Drug Design (Credits: 04)	[CO.1] Concepts of molecular modelling, computer hardware and software, and the molecular modelling literature. [CO.2] Force fields including bond stretching, angle bending, non-bonded interactions, electrostatic interactions, van der Waals Interactions and H-bonding [CO.3] Energy minimization and computer

		<p>Simulation</p> <p>[CO.4] Molecular dynamics & Monte Carlo simulation.</p> <p>[CO.5] Structure prediction and drug design, predicting protein structures by 'Threading', molecular docking, drug discovery – chemoinformatics – QSAR.</p>
5(b)	<p>DCL-306: Molecular Modelling Lab (Credits: 02)</p>	<p>[CO.1] To use various softwares including ChemSketch, ArgusLab (www.planaria-software.com), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer, Hyperchem.</p> <p>[CO.2] To compare the optimized C-C bond lengths and visualize the molecular orbitals.</p> <p>[CO.3] To carry out conformational analysis of simple unsaturated organic molecules and determine the enthalpy of isomerization of <i>cis</i> and <i>trans-isomers</i> of such compounds.</p> <p>[CO.4] To compare the shapes of the simple organic molecules, and show how the shapes affect the boiling points.</p> <p>[CO.5] To visualize the electron density and electrostatic potential maps for diatomic inorganic compounds.</p> <p>[CO.6] To build and minimize organic compounds</p> <p>[CO.7] To determine the heat of hydration of ethylene, and compute the resonance energy of benzene</p>
6(a)	<p>CYD-351: Discipline Specific Elective: Industrial Chemicals and Environment (Credits: 04)</p>	<p>[CO.1] Large scale production, uses, storage and hazards in handling of industrial gases and inorganic chemicals</p> <p>[CO.2] Preparation of metals and ultrapure metals for semiconductor technology</p> <p>[CO.3] Air pollutants and their impact on environment</p> <p>[CO.4] Water pollutants and their impact on environment</p> <p>[CO.5] Water purification methods and industrial waste management</p> <p>[CO.6] Coal, petrol and natural gas, nuclear fuels as sources of energy and related aspects of pollution</p> <p>[CO.7] Biocatalysis and its importance in green chemistry and chemical industry</p>
6(b)	<p>DCL-351: Environmental and Industrial Chemistry Lab (Credits: 02)</p>	<p>[CO.1] To analyse water or aqueous samples and determine (i) dissolved oxygen, (ii) dissolved CO₂, (ii) chemical oxygen demand (COD), biological oxygen demand (BOD), (iii) content of chloride, sulphate, carbonate (CO₃²⁻) and bicarbonate (HCO₃⁻) ions, (iv) salinity and total alkalinity of such water samples.</p>

		<p>[CO.2] To estimate SPM in air samples</p> <p>[CO.3] To determine percentage of available chlorine in bleaching powder.</p> <p>[CO.4] Some of the common bio-indicators of pollution.</p> <p>[CO.5] To prepare and synthesize borax/boric acid.</p>
7	<p>CYD-352: Discipline Specific Elective: Research Methodology for Chemistry (Credits: 06)</p>	<p>[CO.1] Printed sources of information for literature survey, digital sources of information for literature survey, and information technology and library resources</p> <p>[CO.2] Methods of scientific research and writing scientific papers, writing ethics, and avoiding plagiarism.</p> <p>[CO.3] 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.</p> <p>[CO.4] Data analysis, the investigative approach, and analysis and presentation of data</p> <p>[CO.5] Basic fundamentals of electronic circuits and their components used in circuits of common instruments like spectrophotometers.</p>

Theory and lab course will be offered in combination. Course 1(a) will be offered in combination with 1(b). Course 2(a) will be offered in combination with 2(b). Course 3(a) will be offered in combination with 3(b). Course 4(a) will be offered in combination with 4(b). Course 5(a) will be offered in combination with 5(b). Course 6(a) will be offered in combination with 6(b).

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**OUTCOMES OF COURSES
IN
SEVENTH SEMESTER**

Course Type	Course Code and Title	Course Outcome: <i>After completing the course, students will be able to understand:</i>
Core	CYC-401: Structure and Reactivity of Organic Molecules	[CO.1] Conformations and reactivities of cyclohexane and its derivatives. [CO.2] Various models to predict stereochemical outcomes of nucleophilic additions to carbonyl compounds. [CO.3] Thermodynamics and kinetics aspects of a chemical reactions. [CO.4] Various methods for elucidation of reaction mechanism. [CO.5] Different types of catalysis in organic reactions.
Core	CYC-402: Thermodynamics and Interfaces	[CO.1] Understand the concept of classical and statistical thermodynamics, Maxwell Boltzmann, Bose-Einstein, Fermi-Dirac statistics and different partition functions [CO.2] Surface and interfacial phenomenon and their thermodynamics [CO.3] BET Isotherm and its applications [CO.4] Thermodynamics of ionic systems and calculation of energy of interactions in ionic systems
Core	CYC-403: Solid State Chemistry	[CO.1] Crystal structure and symmetry in the crystalline state [CO.2] Applications of XRD in determine crystal structure and phase of a solid material [CO.3] Hard sphere model, structures derived from HCP and CCP packing [CO.4] Bonding in solids and Band theory [CO.5] Properties of solids
Core	CYC-404: Structure and Properties of Metal Complexes	[CO.1] Stereochemistry and bonding in inorganic compounds of main group elements [CO.2] Metal-ligand bonding and molecular orbital theory [CO.3] Metal-ligand equilibria in solution [CO.4] Electronic spectra of coordination compounds [CO.5] Magnetic properties of transition metal complexes
Core	CYC-405: Instrumental Methods of Analysis-I	[CO.1] Basic concepts of qualitative and quantitative analysis [CO.2] Principles and instrumentation of various separation techniques such as liquid chromatography, gas chromatography and electrophoresis [CO.3] Principles and instrumentation of molecular (UV- vs and infrared) spectroscopy, and atomic spectroscopy [CO.4] Principles and instrumentation of electroanalytical methods (such as voltammetry and potentiometry) [CO.3] Principles and instrumentation of thermal methods e.g., TGA, DSC and DTA
Core	CYL-406: Inorganic Chemistry	[CO.1] To perform the experiments in the laboratory for carrying out semi-micro qualitative analysis of inorganic

	Lab-I	ions [CO.2] To perform the experiments in the laboratory for carrying out gravimetric analysis and complexometric titrations to determine the metal content [CO.3] To perform the experiments in the laboratory for synthesizing inorganic coordination compounds
Core	CYL-407: Organic Chemistry Lab-I	[CO.1] To perform the experiments in the laboratory for carrying out the separation of organic mixtures using thin layer chromatography [CO.2] To perform the experiments in the laboratory for carrying out organic chemical transformations such as Diels-Alder reaction, oxidation reactions and reduction reactions [CO.3] To perform the experiments in the laboratory for synthesizing organic compounds
Core	CYL-408: Physical Chemistry Lab-I	[CO.1] To plot and analyse the phase diagram [CO.2] To carry out the electrochemical analysis and its application in understanding the thermodynamics of the given systems. [CO.3] To experimentally determine the rate of reaction of sugars using polarimeter [CO.4] The magnetic and electric properties of the materials



**OUTCOMES OF COURSES
IN
EIGHTH SEMESTER**

Course Type	Course Code and Title	Course Outcome: <i>After completing the course, students will be able to understand:</i>
Core	CYC– 451: <i>Pericyclic and Organic Photochemistry</i>	[CO.1] Classifications of pericyclic reactions, molecular orbital symmetry and frontier molecular orbital concepts. [CO.2] Different electrocyclic reactions with even numbers of electron participation. [CO.3] Various types of sigmatropic rearrangements in pericyclic reactions. [CO.4] Other different types of photochemical reactions in organic chemistry.
Core	CYC– 452: <i>Reagents and Reactions in Organic Chemistry</i>	[CO.1] Various reagents in organic reactions and functional group transformations. [CO.2] Methods for C–C, C–N, C–O single bonds formation. [CO.3] Various models for stereochemical aspects of nucleophilic addition to carbonyl compounds. [CO.3] Methods for C–C, C–N, C–O multiple bonds formations.
Core	CYC– 453: <i>Kinetics and Photochemistry</i>	[CO.1] Chemical kinetics of simple and complex reactions [CO.2] Analysis techniques for fast reactions [CO.3] Kinetics of reactions in solution phase [CO.4] Different theoretical constructs for reaction rate [CO.5] Electrochemistry of ions in solution [CO.6] Electrode-electrolyte interface and different electrochemical processes [CO.7] Photochemical and photo physical processes [CO.8] Radiation chemistry and different dosimeters
Core	CYC– 454: <i>Inorganic Biochemistry and Reaction Mechanism</i>	[CO.1] Reaction mechanism of transition metal complexes [CO.2] Electron transfer reactions [CO.3] Photochemistry of metal complexes [CO.4] Various aspects of inorganic biochemistry [CO.5] Chemical toxicity and metallotherapy
Core	CYC–455: <i>Instrumental Methods of Analysis- II</i>	[CO.1] Principles, instrumentation and applications of vibrational, electron spin resonance (ESR), nuclear magnetic resonance (NMR) and Mossbauer spectroscopy [CO.2] Principles and instrumentation of mass spectrometry [CO.3] Principles and instrumentation of x-ray diffraction techniques [CO.4] Radiochemical methods
Core	CYL–456: <i>Inorganic Chemistry Lab-II</i>	[CO.1] To perform the experiments in the laboratory for quantitative estimation of metal (e.g., nickel) using spectrophotometric methods [CO.2] To interpret and analyse the electronic spectra of complex inorganic ions [CO.3] To perform the experiments in the laboratory for synthesizing inorganic coordination compounds (metal complexes with ligands) and interpret their electronic spectra
Core	CYL–457: <i>Organic Chemistry Lab-II</i>	[CO.1] To perform the experiments in the laboratory for carrying out organic chemical transformations such as Cannizaro reaction and Fischer Indole synthesis [CO.2] To perform the experiments in the laboratory for

		synthesizing specific and important organic compounds
Core	CYL-458: <i>Physical Chemistry Lab-II</i>	[CO.1] To design and execute experiments to study the kinetics of various reactions and the factors effecting the rate of reactions. [CO.2] To use spectrophotometers for the quantitative applications.



**OUTCOMES OF COURSES
IN
NINTH SEMESTER**

Course Type	Course Code and Title	Course Outcome: <i>After completing the course, students will be able to understand:</i>
Core	CYL-501: Inorganic Chemistry Lab-III	[CO.1] To perform the experiments in the laboratory for carrying out qualitative and/or quantitative analysis of metals using spectrophotometric methods, flame photometry and atomic absorption spectroscopy [CO.2] To perform the experiments in the laboratory for carrying out preparation of inorganic coordination compounds.
Core	CYL-502: Organic Chemistry Lab-III	[CO.1] To perform the experiments in the laboratory for carrying out separation of binary mixtures of organic compounds using column chromatography [CO.2] To interpret and analyse the ¹ H and ¹³ C NMR spectra to elucidate the structures of organic compounds [CO.3] To perform the experiments in the laboratory for carrying out organic chemical reactions (such as allylation, esterification and catalytic oxidation) and analyse the products using gas chromatography [CO.4] To perform the experiments in the laboratory for carrying out the synthesis of some peculiar organic compounds such as luminol, anthracene and 4-cyano-2-aminophenol [CO.5] To perform the experiments in the laboratory for determining the quantity of aspirin in the given solution [CO.5] To perform the experiments in the laboratory for estimating the quantity of glucose in the given solution
Core	CYL-503: Physical Chemistry Lab-III	[CO.1] To design and execute experiments to study the surface chemistry of surfactant, micelles and colloidal systems using different techniques. [CO.2] To measure refractive index and analyse the data for quantitative analysis. [CO.3] To carry out electrochemical analysis for quantitation.
DSE	CME-503: Green Chemistry	[CO.1] Green chemistry, and its need, goals, limitations and principles [CO.2] Alternate routes for the green synthesis of some organic compounds [CO.3] Use of microwaves as the source of energy for carrying out the reactions in water [CO.4] Use of ultra sound for performing reactions in water [CO.5] Future trends in green chemistry
DSE	COE-503: Organic Structure Determination	[CO.1] 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] The principles and applications of 2D-NMR spectroscopic techniques in the structure elucidation
DSE	COE-506: Organic Synthesis Lab	[CO.1] To perform experiments in the laboratory to carry out separation of mixture of organic compounds using liquid-liquid extraction [CO.2] To perform experiments in the laboratory to carry out

		<p>multi-step organic synthesis</p> <p>[CO.3] To perform experiments in the laboratory to explore applications of co-enzymes in organic synthesis</p> <p>[CO.4] To perform experiments in the laboratory to carry out isolation of natural products and their characterization</p> <p>[CO.5] To perform experiments in the laboratory to generate nucleophiles and use them in nucleophilic substitution reactions of alkyl halides</p>
DSE	CPE-506: Advanced Physical Chemistry Lab	<p>[CO.1] To design and execute experiments to study the kinetics of reactions under different experimental conditions.</p> <p>[CO.2] To work with sol and gel systems and their viscoelastic properties.</p> <p>[CO.3] To carry out electrochemical analysis for determining thermodynamic parameters.</p> <p>[CO.4] To record and analyse fluorescence spectra of nanomaterials.</p> <p>[CO.5] To record and analyse electronic spectra of nanomaterials and correlate it with structural properties of the same.</p>
DSE	COE-507: Medicinal Chemistry	<p>[CO.1] Drugs, and intermolecular interactions</p> <p>[CO.2] Drug targets including proteins, enzymes and receptors, their structures and functions</p> <p>[CO.3] Concepts of pharmacokinetic and pharmacodynamics</p> <p>[CO.4] Enzymes as drug targets, receptors as drug targets, and nucleic acids as drug targets</p> <p>[CO.5] Drug discovery, design, and development</p> <p>[CO.6] Identification of the structure–activity relationships (SARs), and the pharmacophore in the drug design</p> <p>[CO.7] Ways to improve target interactions (pharmacodynamics) and improve pharmacokinetic properties.</p> <p>[CO.8] Preclinical trials and significance of patent on the drug</p>

*DSE: *Discipline Specific Elective; These courses are chosen by the students from the list of Discipline Specific Elective (DSE) Courses given in Table 4 on the succeeding page.*

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**OUTCOMES OF COURSES
IN
TENTH SEMESTER**

Course Type	Course Code and Title	Course Outcome: <i>After completing the course, students will be able to understand:</i>
Core	CYC- 551: Thesis/Dissertation	To carry out research (experimental or computational) work and writing the report, article and thesis



**OUTCOMES OF DISCIPLINE SPECIFIC ELECTIVE COURSES
IN
NINTH SEMESTER**

Table 4. Discipline Specific Elective Courses for 9th Semester		
S.No.	<i>Course Code and Title</i>	After completion of the course, the students will be able to understand:
1.	Frontiers in Bioinorganic Chemistry (Credits: 03)	[CO.1] Homeostatic mechanism in cells [CO.2] Metal ion transport and assembly of metalloproteins [CO.3] Iron, molybdenum and tungsten in biology [CO.4] Diseases due to metal ions and biomineralization
2.	Inorganic Photochemistry (Credits: 03)	[CO.1] Concepts of photochemistry and properties of excited states [CO.2] Excited states of metal complexes and ligand field photochemistry [CO.3] Redox reactions by excited metal complexes [CO.4] Metal complexes sensitizers
3.	Supramolecular Chemistry (Credits: 03)	[CO.1] Supramolecular chemistry and types of noncovalent interactions [CO.2] Supramolecular chemistry in biological processes [CO.3] Synthesis of supramolecules [CO.4] Physical methods in supramolecular chemistry
4.	Chemistry of Natural Products (Credits: 03)	[CO.1] Natural products, their classification and methods of synthesis and biosynthesis [CO.2] Chemical composition, structure and functions of lignin and pectin [CO.3] Carbohydrates, their classification and biological oxidation [CO.4] Classification, nomenclature, general methods of structure determination and chemistry of terpenoids, pyrethroids and rotenoids [CO.5] Biosynthesis of natural products
5.	Organic Structure Determination (Credits: 03)	[CO.1] 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] The principles and applications of 2D-NMR spectroscopic techniques in the structure elucidation
6.	Modern Organic Synthetic Methods (Credits: 03)	[CO.1] Various important oxidation reactions and name reactions [CO.2] Protection and deprotection of functional groups [CO.3] Retrosynthetic analysis
7.	Total Organic Synthesis (Credits: 03)	[CO.1] Basic Concepts of Total Synthesis [CO.2] Total Synthesis of cubane, endiandric acids, prostaglandins, triquinanes, longifolene, penicillin, steroids (estrone, progesterone & cholesterol), perhydrohistrionicotoxin, methylhomosecodaphnyllane, quinine, yohimbine, reserpine, strychnine, morphine and taxol [CO.3] Total Syntheses of epothilones and eleutherobin
8.	Organic Synthesis Lab (Credits: 03)	[CO.1] To perform experiments in the laboratory to carry out separation of mixture of organic compounds

		<p>using liquid-liquid extraction</p> <p>[CO.2] To perform experiments in the laboratory to carry out multi-step organic synthesis</p> <p>[CO.3] To perform experiments in the laboratory to explore applications of co-enzymes in organic synthesis</p> <p>[CO.4] To perform experiments in the laboratory to carry out isolation of natural products and their characterization</p> <p>[CO.5] To perform experiments in the laboratory to generate nucleophiles and use them in nucleophilic substitution reactions of alkyl halides</p>
9.	Medicinal Chemistry (Credits: 03)	<p>[CO.1] Drugs, and intermolecular interactions</p> <p>[CO.2] Drug targets including proteins, enzymes and receptors, their structures and functions</p> <p>[CO.3] Concepts of pharmacokinetic and pharmacodynamics</p> <p>[CO.4] Enzymes as drug targets, receptors as drug targets, and nucleic acids as drug targets</p> <p>[CO.5] Drug discovery, design, and development</p> <p>[CO.6] Identification of the structure–activity relationships (SARs), and the pharmacophore in the drug design</p> <p>[CO.7] Ways to improve target interactions (pharmacodynamics) and improve pharmacokinetic properties.</p> <p>[CO.8] Preclinical trials and significance of patent on the drug</p>
10	Biophysical Chemistry (Credits: 03)	<p>[CO.1] Biological cell and its constituents</p> <p>[CO.2] Bioenergetics and statistical mechanics in biopolymers</p> <p>[CO.3] Biopolymer interactions</p> <p>[CO.4] Thermodynamics and molecular weight of biopolymers</p> <p>[CO.5] Transport of ions through cell membranes</p>
11	Advance Quantum Chemistry (Credits: 03)	<p>[CO.1] Born Oppenheimer approximation</p> <p>[CO.2] Hartree-Fock method for the solution of Schrodinger equation</p> <p>[CO.3] Models of chemical bonding-Molecular orbital (MO) and Valence bond (VB) theory</p> <p>[CO.4] Hückel π-electron theory and The Pariser-Parr-Pople Method and The CNDO Method.</p>
12.	Solid State Chemistry and Applications (Credits: 03)	<p>[CO.1] Crystal structure of inorganic compounds</p> <p>[CO.2] Defect structure applications of defects in non-stoichiometric compounds.</p> <p>[CO.3] Solid state reactions and the methods to carry out these reactions.</p> <p>[CO.4] Methods of synthesis of nanomaterials and conducting polymers.</p> <p>[CO.5] Intercalation chemistry and the applications of mesoporous materials in heterogeneous catalysis in chemical synthesis.</p> <p>[CO.6] Advanced characterization techniques and their applications.</p>

13.	Advanced Surface and Colloidal Chemistry (Credits: 03)	[CO.1] Surfactants, micelles and their physicochemical properties. [CO.2] Membranes and their applications in fuel cells [CO.3] The importance of adsorption process and catalytic activity at the solid surfaces. [CO.4] Origin and stability of colloidal systems and electric double layer, DLVO theory and Smoluchowski theory. [CO.5] Macromolecules and methods of determination of their molecular weights experimentally
14.	Advanced Physical Chemistry (Credits: 03)	[CO.1] Advanced chemical kinetics [CO.2] Statistical mechanics and irreversible thermodynamics [CO.3] Advanced quantum chemistry
15.	Advanced Physical Chemistry Lab (Credits: 03)	[CO.1] To design and execute experiments to study the kinetics of reactions under different experimental conditions. [CO.2] To work with sol and gel systems and their viscoelastic properties. [CO.3] To carry out electrochemical analysis for determining thermodynamic parameters. [CO.4] To record and analyse fluorescence spectra of nanomaterials. [CO.5] To record and analyse electronic spectra of nanomaterials and correlate it with structural properties of the same.
16.	Environmental Pollutants and Analysis (Credits: 03)	[CO.1] Water pollution, air pollution and soil pollution [CO.2] Pollutants and their analysis
17.	Macromolecules and Nanomaterials (Credits: 03)	[CO.1] Surfactants, micelles and their physicochemical properties. [CO.2] Applications of micelles. [CO.3] Concept of conducting polymers and their applications. [CO.4] Membranes and their applications in separation/extraction techniques. [CO.5] Biomedical applications of polymers [CO.6] Nanomaterials and their methods of synthesis. [CO.7] Common characterization techniques used for studying physical and chemical properties of nanomaterials
18.	Green Chemistry (Credits: 03)	[CO.1] Green chemistry, and its need, goals, limitations and principles [CO.2] Alternate routes for the green synthesis of some organic compounds [CO.3] Use of microwaves as the source of energy for carrying out the reactions in water [CO.4] Use of ultra sound for performing reactions in water [CO.5] Future trends in green chemistry

CYC-101: Inorg. Chem. I: Atomic Structure & Chemical Bonding

Atomic Structure:

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2 . Quantum numbers and their significance.

Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of s , p , d and f orbitals. Contour boundary and probability diagrams.

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

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.

(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table; (b) Atomic radii (van der Waals); (c) Ionic and crystal radii; (d) Covalent radii (octahedral and tetrahedral) (e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy; (f) Electron gain enthalpy, trends of electron gain enthalpy; (g) 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.

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.

Oxidation-Reduction:

Redox equations, Standard Electrode Potential and its application to inorganic reactions. Principles involved in volumetric analysis to be carried out in class.

CYL-101: Titrimetric Analysis Lab

Program:	Integrated M.Sc.	Credits:	02
Type:	Core Course	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYC-101: Inorg. Chem. I: Atomic Structure & Chemical Bonding”		

(A) Titrimetric Analysis

- (i) Calibration and use of apparatus
- (ii) Preparation of solutions of different Molarity/Normality of titrants

(B) Acid-Base Titrations

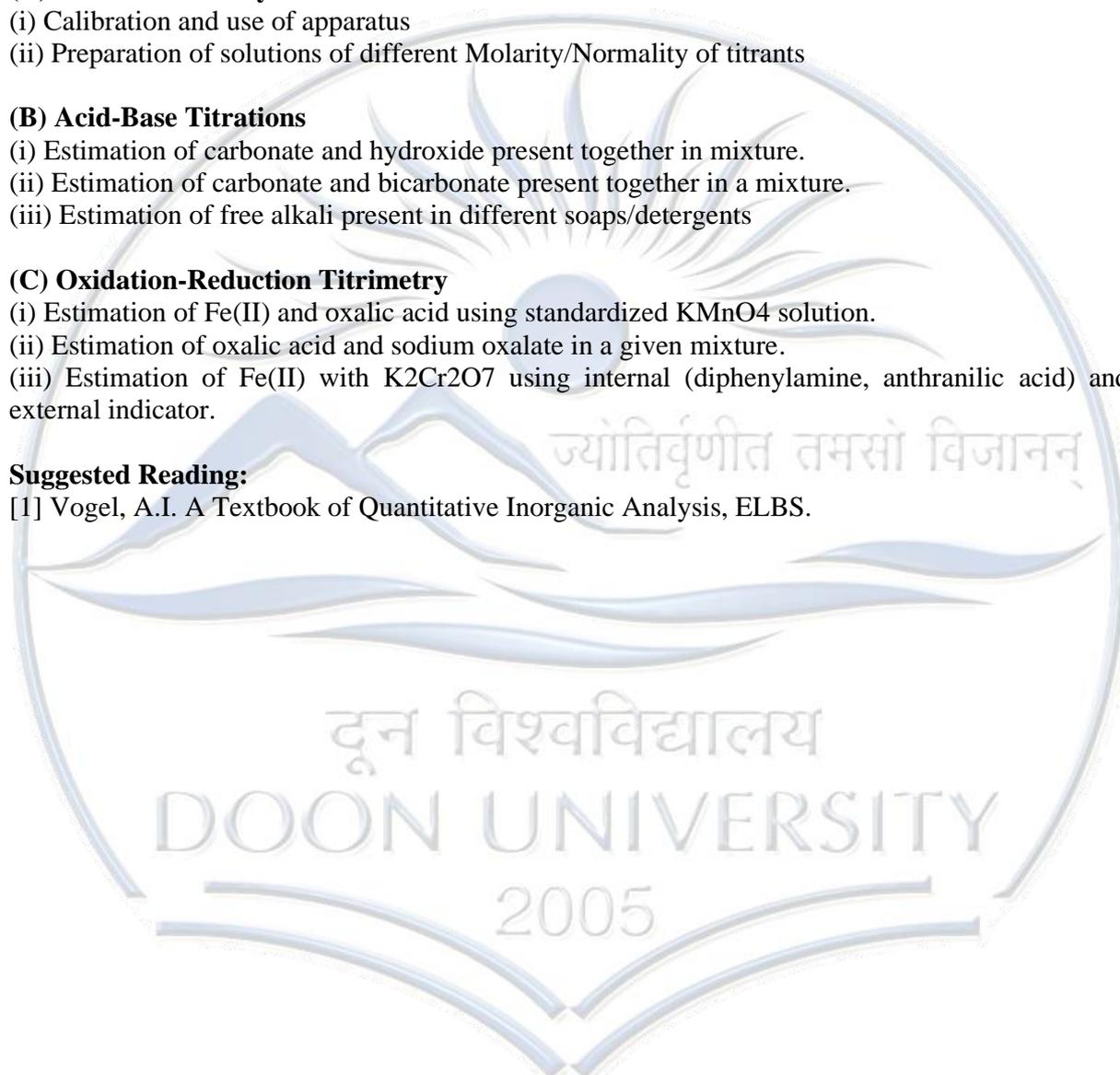
- (i) Estimation of carbonate and hydroxide present together in mixture.
- (ii) Estimation of carbonate and bicarbonate present together in a mixture.
- (iii) Estimation of free alkali present in different soaps/detergents

(C) Oxidation-Reduction Titrimetry

- (i) Estimation of Fe(II) and oxalic acid using standardized KMnO₄ solution.
- (ii) Estimation of oxalic acid and sodium oxalate in a given mixture.
- (iii) Estimation of Fe(II) with K₂Cr₂O₇ using internal (diphenylamine, anthranilic acid) and external indicator.

Suggested Reading:

- [1] Vogel, A.I. A Textbook of Quantitative Inorganic Analysis, ELBS.



CYC-102: Phys. Chem. I: States of Matter & Ionic Equilibrium**Gaseous State:**

Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; 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.

Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor, Z , and its variation with pressure for different gases. Causes of deviation from ideal behaviour. Van der Waals equation of state, its derivation and application in explaining real gas behaviour, mention of other equations of state (Berthelot, Dieterici); virial equation of state; van der Waals equation expressed in virial form and calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states.

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.

Solid state:

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl. Defects in crystals. Glasses and liquid crystals.

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.

Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid–base indicators; selection of indicators and their limitations.

Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants.

CYL-102: Physicochemical Analysis Lab

Program:	Integrated M.Sc.	Type: Core Course
Credits:	02	Contact Hours: 04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYC-102: Phys. Chem. I: States of Matter & Ionic Equilibrium”	

[1] Surface tension measurements.

- a. Determine the surface tension by (i) drop number (ii) drop weight method.
- b. Study the variation of surface tension of detergent solutions with concentration.

[2] Viscosity measurement using Ostwald’s viscometer.

- a. Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.
- b. Study the variation of viscosity of sucrose solution with the concentration of solute.

[3] Indexing of a given powder diffraction pattern of a cubic crystalline system.

[4] pH metry

- a. Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
- b. Preparation of buffer solutions of different pH
 - i. Sodium acetate-acetic acid
 - ii. Ammonium chloride-ammonium hydroxide
- c. pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.
- d. Determination of dissociation constant of a weak acid.

Any other experiment carried out in the class.

Suggested Readings:

- [1] Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- [2] Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
- [3] Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).

First Semester

CYG-101: Generic Chem.:
Atomic Structure, Bonding, General Organic Chemistry, & Aliphatic Hydrocarbons

Section A: Inorganic Chemistry-1

(30 Lectures)

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 hydrogenic 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)

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)

Section B: Organic Chemistry-1

(30 Lectures)

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.

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)

Aliphatic 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, oxymercuration-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 . (12 Lectures)

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 Alexander: *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] T. W. Graham Solomon: *Organic Chemistry*, John Wiley and Sons.
- [6] Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
- [7] E. L. Eliel: *Stereochemistry of Carbon Compounds*, Tata McGraw Hill.
- [8] I. L. Finar: *Organic Chemistry (Vol. I & II)*, E. L. B. S.
- [9] R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
- [10] Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand

GCL-101: Inorg. and Org. Chemical Analysis Lab

Program: Integrated M.Sc. **Semester:** First

Type: *Generic Elective Course* **Credits:** 02

Contact Hours: 04 × 15 (04 Hr/Week)

Corresponding Theory Course: To be offered in combination with the theory course titled “CYG-101: *Generic Chem. : Atomic Structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons*”

Section A: Inorganic Chemistry - Volumetric Analysis

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with KMnO_4 .
3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO_4 .
4. Estimation of Fe (II) ions by titrating it with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using $\text{Na}_2\text{S}_2\text{O}_3$.

Section B: Organic Chemistry

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)
2. Separation of mixtures by Chromatography: Measure the R_f value in each case (combination of two compounds to be given)
 - (a) Identify and separate the components of a given mixture of 2 amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by paper chromatography
 - (b) Identify and separate the sugars present in the given mixture by paper chromatography.

Reference Books:

- [1] Vogel's Qualitative Inorganic Analysis, A.I. Vogel, Prentice Hall, 7th Edition.
- [2] Vogel's Quantitative Chemical Analysis, A.I. Vogel, Prentice Hall, 6th Edition.
- [3] Textbook of Practical Organic Chemistry, A.I. Vogel, Prentice Hall, 5th edition.
- [4] Practical Organic Chemistry, F. G. Mann. & B. C. Saunders, Orient Longman, 1960.

CYC-151: Org. Chem. I: Basics & Hydrocarbons**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.

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.

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.

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.

CYL-151: Organic Compounds Purification Lab

Program:	Integrated M.Sc.	Semester:	Second
Type:	Core Course		
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYC-151: Org. Chem. I: Basics and Hydrocarbons”		

- [1] Checking the calibration of the thermometer
- [2] Purification of organic compounds by crystallization using the following solvents: (a) *Water*, (b) *Alcohol* and (c) *Alcohol-Water*
- [3] Determination of the melting points of above compounds and unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)
- [4] Effect of impurities on the melting point – mixed melting point of two unknown organic compounds
- [5] Determination of boiling point of liquid compounds. (boiling point lower than and more than 100 °C by distillation and capillary method)
- [6] Chromatography
 - a. *Separation of a mixture of two amino acids by ascending and horizontal paper chromatography*
 - b. *Separation of a mixture of two sugars by ascending paper chromatography*
 - c. *Separation of a mixture of o-and p-nitrophenol or o-and p-aminophenol by thin layer chromatography (TLC)*

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)

CYC-152: Phys. Chem. II: Chemical Thermodynamics & its Applications

Chemical Thermodynamics:

Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics.

First law: Concept of heat, q , work, w , internal energy, U , and statement of first law; enthalpy, H , relation between heat capacities, calculations of q , w , U and H for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions.

Thermochemistry: Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions. Adiabatic flame temperature, explosion temperature.

Second Law: Concept of entropy; thermodynamic scale of temperature, statement of the second law of thermodynamics; molecular and statistical interpretation of entropy. Calculation of entropy change for reversible and irreversible processes.

Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules.

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.

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.

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 K_p , K_c and K_x . Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

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.

CYL-152: Thermochemistry Lab

Program:	Integrated M.Sc.	Semester:	Second
Course Title:	<i>Thermochemistry Lab</i>		
Course Code:	CYL-152	Type:	Core Course
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYC-152: <i>Phys. Chem. II: Chemical Thermodynamics and Its Applications</i> ”		

Thermochemistry

- Determination of 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).
- Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
- Calculation of the enthalpy of ionization of ethanoic acid.
- Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.
- Determination of 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.
- Determination of enthalpy of hydration of copper sulphate.
- Study of the solubility of benzoic acid in water and determination of ΔH .

Any other experiment carried out in the class.

Suggested Readings:

- [1] Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- [2] Athawale, V. D. & Mathur, P. *Experimental Physical Chemistry* New Age International: New Delhi (2001).

CYG-151: Generic Chem.: Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I

Section A: Physical Chemistry-1

(30 Lectures)

Chemical Energetics

(10 Lectures)

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.

Chemical Equilibrium:

(8 Lectures)

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

Ionic Equilibria:

(12 Lectures)

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.

Section B: Organic Chemistry-2

(30 Lectures)

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

Aromatic hydrocarbons:

(8 Lectures)

Preparation (Case benzene): from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid.

Reactions: (Case benzene): 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).

Alkyl and Aryl Halides

Alkyl Halides (Upto 5 Carbons): Types of Nucleophilic Substitution (SN_1 , SN_2 and SN_i) 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 $\text{NaNH}_2/\text{NH}_3$).

Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides. (8 Lectures)

Alcohols, Phenols and Ethers (Upto 5 Carbons)

Alcohols:

Preparation: Preparation of 1^o, 2^o and 3^o 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.

Aldehydes and ketones (aliphatic and aromatic): (Formaldehyde, acetaldehyde, acetone and benzaldehyde).

Preparation: from acid chlorides and from nitriles.

Reactions – Reaction with HCN, ROH, NaHSO_3 , $\text{NH}_2\text{-G}$ derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Ponndorf Verley reduction. (14 Lectures)

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

GCL-151: Basic Physical and Organic Chemistry Lab

Program:	Integrated M.Sc.	Semester:	Second
Course Title:	<i>Basic Physical and Organic Chemistry Lab</i>		
Course Code:	<i>GCL-151</i>	Type:	<i>Generic Elective Course</i>
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled " <i>CYG-151: Generic Chem. : Chemical Energetics, Equilibria & Functional Group Org. Chem. I</i> "		

Section A: Physical Chemistry

Thermochemistry

1. Determination of heat capacity of calorimeter for different volumes.
2. Determination of enthalpy of neutralization of HCl with NaOH.
3. Determination of enthalpy of ionization of acetic acid.
4. Determination of integral enthalpy of solution of salts (KNO₃, NH₄Cl).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of ΔH .

Ionic equilibria

pH measurements

- a) Measurement of 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.
- b) Preparation of buffer solutions: (i) Sodium acetate-acetic acid, and (ii) Ammonium chloride-ammonium hydroxide
Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

Section B: Organic Chemistry

1. Purification of organic compounds by crystallization (from water and alcohol) and distillation.
2. Criteria of Purity: Determination of melting and boiling points.
3. Preparations: Mechanism of various reactions involved to be discussed. Recrystallisation, determination of melting point and calculation of quantitative yields to be done.
 - (a) Bromination of Phenol/Aniline
 - (b) Benzoylation of amines/phenols
 - (c) Oxime and 2,4 dinitrophenylhydrazone of aldehyde/ketone

Reference Books

- [1] A.I. Vogel: Textbook of Practical Organic Chemistry, 5th edition, Prentice-Hall.
- [2] F. G. Mann & B. C. Saunders, Practical Organic Chemistry, Orient Longman (1960).
- [3] B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

CYC-201: Inorg. Chem. II: s- and p-Block Elements**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.

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.

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.

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).

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.

CYL-201: Quantitative Inorganic Analysis and Synthesis Lab

Program:	Integrated M.Sc.	Semester:	Third
Course Title:	<i>Quantitative Inorganic Analysis and Synthesis Lab</i>		
Course Code:	CYL-201	Type:	Core Course
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYC-201: Inorg. Chem. II: s- and p-Block Elements”		

[A] Iodo / Iodimetric Titrations

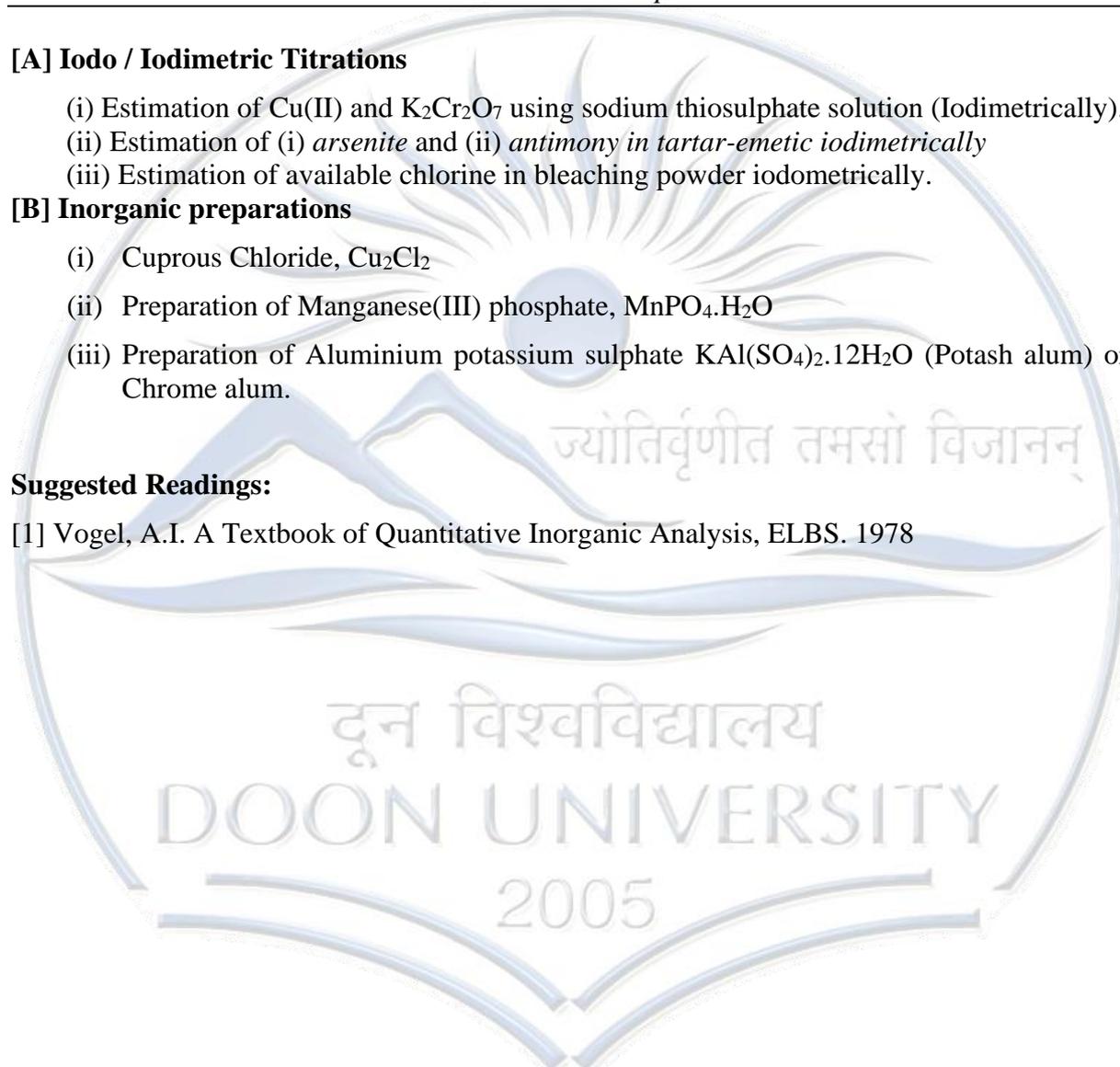
- (i) Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodimetrically).
- (ii) Estimation of (i) *arsenite* and (ii) *antimony in tartar-emetica iodimetrically*
- (iii) Estimation of available chlorine in bleaching powder iodometrically.

[B] Inorganic preparations

- (i) Cuprous Chloride, Cu_2Cl_2
- (ii) Preparation of Manganese(III) phosphate, $MnPO_4 \cdot H_2O$
- (iii) Preparation of Aluminium potassium sulphate $KAl(SO_4)_2 \cdot 12H_2O$ (Potash alum) or Chrome alum.

Suggested Readings:

- [1] Vogel, A.I. A Textbook of Quantitative Inorganic Analysis, ELBS. 1978



CYC-202: Phys. Chem. III: Phase Equilibria & Chemical Kinetics

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 solid-liquid, 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.

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.

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.

Surface chemistry:

Physical adsorption, chemisorption, adsorption isotherms. nature of adsorbed state.

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. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
- [6] Zundhal, S.S. Chemistry concepts and applications Cengage India (2011).
- [7] Ball, D. W. Physical Chemistry Cengage India (2012).
- [8] Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
- [9] Levine, I. N. Physical Chemistry 6th Ed., Tata McGraw-Hill (2011).

CYL-202: Chemical Kinetics Lab

Program:	Integrated M.Sc.	Semester:	Third
Course Title:	<i>Chemical Kinetics Lab</i>		
Course Code:	<i>CYL-202</i>	Type:	Core Course
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled " <i>CYC-202: Phys. Chem. III: Phase Equilibrium and Chemical Kinetics</i> "		

- [I] Determination of critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.
- [II] Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method: (a) simple eutectic and (b) congruently melting systems.
- [III] Distribution of acetic/ benzoic acid between water and cyclohexane.
- [IV] Study the equilibrium of at least one of the following reactions by the distribution method:
- (i) $I_2(aq) + I^- \rightarrow I_3^-(aq)$
- (ii) $Cu^{2+}(aq) + nNH_3 \rightarrow Cu(NH_3)_n$
- [V] Study the kinetics of the following reactions:
- (1) Initial rate method: *Iodide-persulphate reaction*
- (2) Integrated rate method: (a) *Acid hydrolysis of methyl acetate with hydrochloric acid*, and (b) *Saponification of ethyl acetate*.
- (3) Compare the strengths of HCl and H₂SO₄ by studying kinetics of hydrolysis of methyl acetate.
- [VI] Adsorption
- I. Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

Suggested Readings:

- [1] Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- [2] Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
- [3] Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).

CYC-203: Org. Chem. II: Oxygen Containing Functional Groups

Chemistry of Halogenated Hydrocarbons:

Alkyl Halides: Methods of preparation, nucleophilic substitution reactions – S_N^1 , S_N^2 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.

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 $LiAlH_4$

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, $LiAlH_4$, $NaBH_4$, 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.

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 substitution at acyl group - Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmannbromamide degradation and Curtius rearrangement.

Sulphur containing compounds:

Preparation and reactions of thiols, thioethers and sulphonic acids.

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] Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.

Third Semester
CYL-203: Basic Organic Synthesis Lab

Program:	Integrated M.Sc.	Semester:	Third
Course Title:	<i>Basic Organic Synthesis Lab</i>		
Course Code:	CYL-203	Type:	Core Course
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYC-203: Org. Chem. II: Oxygen Containing Functional Groups”		

- [1] Functional group tests for alcohols, phenols, carbonyl and carboxylic acid group.
- [2] Organic preparations:
- (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) Benzoylation 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, p-cresol) 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)*.
 - (v) Selective reduction of *meta* dinitrobenzene to *m*-nitroaniline.
 - (vi) Reduction of *p*-nitrobenzaldehyde by sodium borohydride.
 - (vii) Hydrolysis of amides and esters.
 - (viii) Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.
 - (ix) *S*-Benzylisothiuronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
 - (x) Aldol condensation using either conventional or green method.
 - (xi) Benzil-Benzilic acid rearrangement.
- 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] Generation of nucleophile from substituted thiophenol(s) and its use in nucleophilic substitution reaction of primary alkyl halide (*Incorporated by approval of Academic Counsel in its 25th meeting under Agenda Item No. 2018:25:26 in May 2018*)

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).

CYG-201: Generic Chem.: s- and p-Block Elements, States of Matter and Chemical Kinetics

Section A: Inorganic Chemistry

(30 Lectures)

General Principles of Metallurgy:

(4 Lectures)

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.

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.

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

Section B: Physical Chemistry-3

(30 Lectures)

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. Andrews isotherms of CO_2 .

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).

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)

Solids

Forms of solids. Symmetry elements, unit cells, crystal systems, Bravais lattice types and identification of lattice planes. Laws of Crystallography - Law of constancy of interfacial angles, Law of rational indices. 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.

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).

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.

दून विश्वाविद्यालय
DOON UNIVERSITY
2005

GCL-201: Basic Physical and Inorganic Chemistry Lab

Program:	Integrated M.Sc.	Semester:	Third
Course Title:	<i>Basic Physical and Inorganic Chemistry Lab</i>		
Course Code:	<i>GCL-201</i>	Type:	<i>Generic Elective Course</i>
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled " <i>CYG-201: Generic Chem. : s- and p-Block Elements, States of Matter & Chemical Kinetics</i> "		

Section A: Inorganic Chemistry

Semi-micro qualitative analysis using H₂S of mixtures- not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

Cations : NH₄⁺, Pb²⁺, Ag⁺, Bi³⁺, Cu²⁺, Cd²⁺, Sn²⁺, Fe³⁺, Al³⁺, Co²⁺, Cr³⁺, Ni²⁺, Mn²⁺, Zn²⁺, Ba²⁺, Sr²⁺, Ca²⁺, K⁺

Anions : CO₃²⁻, S²⁻, SO₂⁻, S₂O₃²⁻, NO₃⁻, CH₃COO⁻, Cl⁻, Br⁻, I⁻, NO₃⁻, SO₄²⁻, PO₄³⁻, BO₃³⁻, C₂O₄²⁻, F⁻

(Spot tests should be carried out wherever feasible)

Section B: Physical Chemistry

- (I) Surface tension measurement (use of organic solvents excluded).
- Determination of the surface tension of a liquid or a dilute solution using a stalagmometer.*
 - Study of the variation of surface tension of a detergent solution with concentration.*
- (II) Viscosity measurement (use of organic solvents excluded).
- Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwald's viscometer.*
 - Study of the variation of viscosity of an aqueous solution with concentration of solute.*
- (III) Chemical Kinetics:
Study the kinetics of the following reactions.
- Initial rate method: *Iodide-persulphate reaction.*
 - Integrated rate method: (a) *Acid hydrolysis of methyl acetate with hydrochloric acid,*
(b) *Saponification of ethyl acetate and (c) Compare the strengths of HCl and H₂SO₄ by studying kinetics of hydrolysis of methyl acetate*

Reference Books:

- [1] A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- [2] A.I. Vogel, Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- [3] B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

CYC-251: Inorg. Chem. III: Coordination Chemistry**Coordination Chemistry:**

Werner's theory, valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of $10 Dq$ (Δ_o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of $10 Dq$ (Δ_o , Δ_t). 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.

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)

Lanthanoids and Actinoids:

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

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.

CYL-251: Inorganic Preparation, Separation and Gravimetric Analysis Lab

Program: Integrated M.Sc.	Semester: Fourth
Course Title: <i>Inorganic Preparation, Separation & Gravimetric Analysis Lab</i>	
Course Code: CYL-251	Type: Core Course
Credits: 02	Contact Hours: 04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYC-251: <i>Inorg. Chem. III: Coordination Chemistry</i> ”

Gravimetric Analysis:

- Estimation of nickel (II) using Dimethylglyoxime (DMG).
- Estimation of copper as CuSCN
- Estimation of iron as Fe₂O₃ by precipitating iron as Fe(OH)₃.
- Estimation of Al (III) by precipitating with oxine and weighing as Al(oxine)₃ (aluminium oxinate).

Inorganic Preparations:

- Tetraamminecopper (II) sulphate, [Cu(NH₃)₄]SO₄.H₂O
- Cis* and *trans* K[Cr(C₂O₄)₂. (H₂O)₂] Potassium dioxalatochromate (III)
- Tetraamminecarbonatocobalt (III) ion
- Potassium tris(oxalato)ferrate(III)

Chromatography of metal ions

Principles involved in chromatographic separations. Paper chromatographic separation of following metal ions:

- Ni (II) and Co (II)
- Fe (III) and Al (III)

Reference Book:

- Vogel, A.I. A text book of Quantitative Analysis, ELBS 1986.

CYC-252: Org. Chem. III: Heterocyclic Chemistry**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.

Polynuclear Hydrocarbons

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

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.

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.

Terpenes

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

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).

CYL-252: Organic Qualitative Analysis Lab

Program:	Integrated M.Sc.	Semester:	Fourth
Course Title:	<i>Organic Qualitative Analysis Lab</i>		
Course Code:	CYL-252	Type:	Core Course
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYC-252: Org. Chem. III: Heterocyclic Chemistry”		

- [1] Detection of extra elements.
- [2] Functional group test for nitro, amine and amide groups.
- [3] Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols and carbonyl compounds)
- [4] Reaction of amines with carbonyl compound derivatives of different polyaromatic hydrocarbons and heterocyclic compounds. (*Incorporated by approval of Academic Counsel in its 25th meeting under Agenda Item No. 2018:25:27 in May 2018*)

Reference Books

- [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).

CYC-253: Phys. Chem. IV: Electrochemistry**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.

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 $\text{SbO/Sb}_2\text{O}_3$ 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).

Electrical & Magnetic Properties of Atoms and Molecules

Basic ideas of electrostatics, Electrostatics of dielectric media, Clausius-Mosotti equation, Lorenz-Laurentz equation, Dipole moment and molecular polarizabilities and their measurements. Diamagnetism, paramagnetism, magnetic susceptibility and its measurement, molecular interpretation.

Suggested Readings:

- [1] Atkins, P.W & Paula, J.D. Physical Chemistry, 9th Ed., Oxford University Press (2011).
- [2] Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
- [3] Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
- [4] Barrow, G. M., Physical Chemistry 5th Ed., Tata McGraw Hill: New Delhi (2006).
- [4] Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- [5] Rogers, D. W. Concise Physical Chemistry Wiley (2010).
- [6] Silbey, R. J.; Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed., John Wiley & Sons, Inc. (2005).

Fourth Semester
CYL-253: Electrochemistry Lab

Program: Integrated M.Sc. **Semester:** Fourth
Course Title: *Electrochemistry Lab*
Course Code: CYL-253 **Type:** Core Course
Credits: 02 **Contact Hours:** 04 × 15 (04 Hr/Week)
Corresponding Theory Course: To be offered in combination with the theory course titled “CYC-253: *Phys. Chem. IV: Electrochemistry*”

Conductometry

- I. Determination of cell constant
- II. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
- III. Perform the following conductometric titrations:
 - i. *Strong acid vs. strong base*
 - ii. *Weak acid vs. strong base*
 - iii. *Mixture of strong acid and weak acid vs. strong base*
 - iv. *Strong acid vs. weak base*

Potentiometry

- I Perform the following potentiometric titrations:
- i. *Strong acid vs. strong base*
 - ii. *Weak acid vs. strong base*
 - iii. *Dibasic acid vs. strong base*
 - iv. *Potassium dichromate vs. Mohr's salt*

Suggested Readings:

- [1] Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- [2] Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
- [3] Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).

CYG-252: Generic Chem.: Organometallics, Bioinorganic Chemistry, Polymer Hydrocarbons and UV-IR Spectroscopy

Section A: Inorganic Chemistry-4

(30 Lectures)

Chemistry of 3d metals

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

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, $[Co(NH_3)_6]Cl_3$, $Na_3[Co(NO_2)_6]$. (6 Lectures)

Organometallic Compounds

Definition and Classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p and multicentre bonds). Structures of methyl lithium, Zeiss salt and ferrocene. EAN rule as applied to carbonyls. Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d metals. π -acceptor behaviour of carbon monoxide. Synergic effects (VB approach)- (MO diagram of CO can be referred to for synergic effect to IR frequencies). (12 Lectures)

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). (12 Lectures)

Section B: Organic Chemistry-4

(30 Lectures)

Polynuclear and heteronuclear aromatic compounds:

Properties of the following compounds with reference to electrophilic and nucleophilic substitution: Naphthalene, Anthracene, Furan, Pyrrole, Thiophene, and Pyridine. (6 Lectures)

Active methylene compounds:

Preparation: Claisen ester condensation. Keto-enol tautomerism.

Reactions: Synthetic uses of ethylacetoacetate (preparation of non-heteromolecules having upto 6 carbon). (6 Lectures)

Application of Spectroscopy to Simple Organic Molecules

Application of visible, ultraviolet and Infrared spectroscopy in organic molecules. Electromagnetic radiations, electronic transitions, λ_{max} and ϵ_{max} , chromophore, auxochrome, bathochromic and hypsochromic shifts. Application of electronic spectroscopy and Woodward rules for calculating λ_{max} of conjugated dienes and α,β – unsaturated compounds. Infrared radiation and types of molecular vibrations, functional group and fingerprint region. IR spectra of alkanes, alkenes and simple alcohols (inter and intramolecular hydrogen bonding), aldehydes, ketones, carboxylic acids and their derivatives (effect of substitution on $>C=O$ stretching absorptions). (18 Lectures)

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.

GCL-252: Inorg. and Org. Synthesis and Qualitative Analysis Lab

Program:	Integrated M.Sc.	Semester:	Fourth
Course Title:	<i>Inorg. & Org. Synthesis and Qualitative Analysis Lab</i>		
Course Code:	GCL-252	Type:	Generic Elective Course
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYG-252: <i>Generic Chem. : Organometallics, Bioinorganic Chemistry, Polynuclear Hydrocarbons and UV-IR Spectroscopy</i> ”		

Section A: Inorganic Chemistry

- [1] Separation of mixtures by chromatography: Measure the *R_f* value in each case (Combination of two ions to be given).
Paper chromatographic separation of Fe³⁺, Al³⁺ and Cr³⁺ or
Paper chromatographic separation of Ni²⁺, Co²⁺, Mn²⁺ and Zn²⁺
- [2] Preparation of 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, MgCl₂ and LiCl₃.*

Section B: Organic Chemistry

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] A.I. Vogel: Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- [2] A.I. Vogel: Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- [3] A.I. Vogel: Textbook of Practical Organic Chemistry, Prentice Hall, 5th Edn.
- [4] F. G. Mann & B. C. Saunders: Practical Organic Chemistry, Orient Longman (1960).

CYC-301: Org. Chem. IV: Biomolecules**Nucleic Acids:**

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

Amino Acids, Peptides and Proteins:

Amino acids, Peptides and their classification.

α -Amino Acids: Synthesis, ionic properties and reactions. Zwitterions, pK_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

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).

Lipids:

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

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.

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).

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

Fifth Semester

CYL-301: Biochemistry Lab

Program: Integrated M.Sc.	Semester: Fifth (5 th)
Course Title: <i>Biochemistry Lab</i>	
Course Code: <i>CYL-301</i>	Type: Core Course
Credits: 02	Contact Hours: 04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled " <i>CYC-301: Org. Chem. IV: Biomolecules</i> "

- [1] Estimation of glycine by Sorenson's formalin method.
- [2] Study of the titration curve of glycine.
- [3] Estimation of proteins by Lowry's method.
- [4] Study of the action of salivary amylase on starch at optimum conditions.
- [5] Effect of temperature on the action of salivary amylase.
- [6] Saponification value of an oil or a fat.
- [7] Determination of Iodine number of an oil/ fat.
- [8] Isolation and characterization of DNA from onion/ cauliflower/peas.

Suggested Readings:

- [1] Manual of Biochemistry Workshop, 2012, Department of Chemistry, University of Delhi.
- [2] Arthur, I. V. *Quantitative Organic Analysis*, Pearson.

दून विश्वविद्यालय
DOON UNIVERSITY
2005

CYC-302: Phys. Chem. V: Quantum Chemistry & Spectroscopy

Quantum Chemistry

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.

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).

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 (BeH_2 , H_2O) molecules. Qualitative MO theory and its application to AH_2 type molecules.

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.

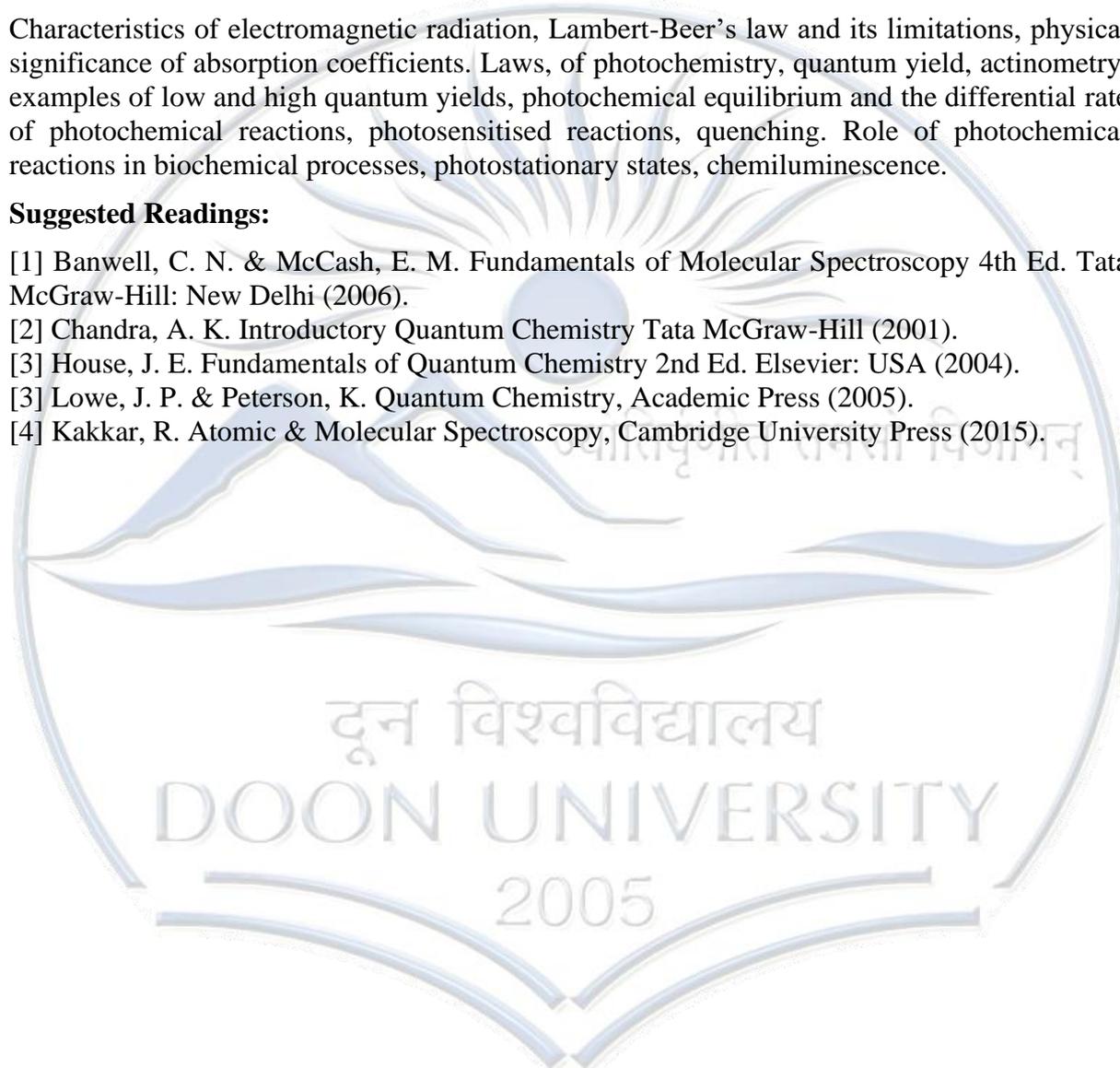
Electron Spin Resonance (ESR) Spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

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.

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).
- [3] Lowe, J. P. & Peterson, K. Quantum Chemistry, Academic Press (2005).
- [4] Kakkar, R. Atomic & Molecular Spectroscopy, Cambridge University Press (2015).



CYL-302: Spectroscopic Analysis Lab

Program:	Integrated M.Sc.	Semester:	Fifth (5 th)
Course Title:	<i>Spectroscopic Analysis Lab</i>		
Course Code:	CYL-302	Type:	Core Course
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYC-302: Phys. Chem. V: Quantum Chemistry & Spectroscopy”		

UV/Visible spectroscopy

- [I] Study the 200-500 nm absorbance spectra of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ (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).
- [II] Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $\text{K}_2\text{Cr}_2\text{O}_7$.
- [III] 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.

Colourimetry

- [I] Verify Lambert-Beer's law and determine the concentration of $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$ in a solution of unknown concentration
- [II] Determine the concentrations of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ in a mixture.
- [III] Study the kinetics of iodination of propanone in acidic medium.
- [IV] Determine the amount of iron present in a sample using 1,10-phenanthroline.
- [V] Determine the dissociation constant of an indicator (phenolphthalein).
- [VI] Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.
- [VII] Analysis of the given vibration-rotation spectrum of $\text{HCl}(\text{g})$

Suggested Readings:

- [1] Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- [2] Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
- [3] Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).

CYC-351: Inorg. Chem. IV: Organometallic Chemistry

Theoretical Principles in Qualitative Analysis (H₂S Scheme)

Basic principles involved in analysis of cations and anions and solubility products, common ion effect. Principles involved in separation of cations into groups and choice of group reagents. Interfering anions (fluoride, borate, oxalate and phosphate) and need to remove them after Group 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.

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.

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

CYL-351: Inorganic Synthesis and Qualitative Analysis Lab

Program:	Integrated M.Sc.	Semester:	Sixth (6 th)
Course Title:	Inorganic <i>Synthesis & Qualitative Analysis Lab</i>		
Course Code:	CYL-351	Type:	Core Course
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYC-351: Inorg. Chem. IV: Organometallic Chemistry”		

Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:

CO_3^{2-} , NO_2^- , S^{2-} , SO_3^{2-} , $\text{S}_2\text{O}_3^{2-}$, CH_3COO^- , F^- , Cl^- , Br^- , I^- , NO_3^- , BO_3^{3-} , $\text{C}_2\text{O}_4^{2-}$, PO_4^{3-} , NH_4^+ , K^+ , Pb^{2+} , Cu^{2+} , Cd^{2+} , Bi^{3+} , Sn^{2+} , Sb^{3+} , Fe^{3+} , Al^{3+} , Cr^{3+} , Zn^{2+} , Mn^{2+} , Co^{2+} , Ni^{2+} , Ba^{2+} , Sr^{2+} , Ca^{2+} , Mg^{2+}

Mixtures should preferably contain one interfering anion, or insoluble component (BaSO_4 , SrSO_4 , PbSO_4 , CaF_2 or Al_2O_3) or combination of anions e.g. CO_3^{2-} and SO_3^{2-} , NO_2^- and NO_3^- , Cl^- and Br^- , Cl^- and I^- , Br^- and I^- , NO_3^- and Br^- , NO_3^- and I^- .

Spot tests should be done whenever possible.

- Measurement of 10 Dq by spectrophotometric method
- Verification of spectrochemical series.
- Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs thermodynamic factors.
- Preparation of acetylacetonato complexes of $\text{Cu}^{2+}/\text{Fe}^{3+}$. Find the λ_{max} of the complex.
- Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetonone, DMG, glycine) by substitution method.

Suggested Readings for both CYC-351 and CYL-351:

- [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*

CYC-352: Org. Chem. V: Carbohydrates, Dyes, Polymers and Basics of Org. Spectroscopy

Organic Spectroscopy

General principles Introduction to absorption and emission spectroscopy.

UV Spectroscopy: Types of electronic transitions, λ_{\max} , 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.

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.

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, Interpretation of NMR spectra of simple compounds. *Applications of IR, UV and NMR for identification of simple organic molecules.*

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.

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.

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.

CYL-352: Organic Synthesis & Qualitative Analysis Lab

Program:	Integrated M.Sc.	Semester:	Sixth (6 th)
Course Title:	<i>Organic Synthesis & Qualitative Analysis Lab</i>		
Course Code:	CYL-352	Type:	Core Course
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYC-351: <i>Org. Chem. V: Carbohydrates, Dyes, Polymers and Basics of Org. Spectroscopy</i> ”		

- [1] Extraction of caffeine from tea leaves.
- [2] Preparation of sodium polyacrylate.
- [3] Preparation of urea formaldehyde.
- [4] Analysis of Carbohydrate: aldoses and ketoses, reducing and non-reducing sugars.
- [5] Qualitative analysis of unknown organic compounds containing monofunctional groups (carbohydrates, aryl halides, aromatic hydrocarbons, nitro compounds, amines and amides) and simple bifunctional groups, for e.g. salicylic acid, cinnamic acid, nitrophenols etc.
- [6] Identification of simple organic compounds by IR spectroscopy and NMR spectroscopy (Spectra to be provided).
- [7] Preparation of methyl orange.

Suggested Readings for CYC-352:

- [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

Suggested Readings for CYL-352:

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

CYG-101: Generic Chem.:

Atomic Structure, Bonding, General Organic Chemistry, & Aliphatic Hydrocarbons

Section A: Inorganic Chemistry-1

(30 Lectures)

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 hydrogenic 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)

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)

Section B: Organic Chemistry-1

(30 Lectures)

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.

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)

Aliphatic 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, oxymercuration-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 . (12 Lectures)

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 Alexander: *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] T. W. Graham Solomon: *Organic Chemistry*, John Wiley and Sons.
- [6] Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
- [7] E. L. Eliel: *Stereochemistry of Carbon Compounds*, Tata McGraw Hill.
- [8] I. L. Finar: *Organic Chemistry (Vol. I & II)*, E. L. B. S.
- [9] R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
- [10] Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand

GCL-101: Inorg. and Org. Chemical Analysis Lab

(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters)

Program: Integrated M.Sc. **Semester:** Generally chosen at First Semester

Type: *Generic Elective Course* **Credits:** 02

Contact Hours: 04 × 15 (04 Hr/Week)

Corresponding Theory Course: To be offered in combination with the theory course titled “*CYG-101: Generic Chem.: Atomic Structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons*”

Section A: Inorganic Chemistry - Volumetric Analysis

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with KMnO_4 .
3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO_4 .
4. Estimation of Fe (II) ions by titrating it with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using $\text{Na}_2\text{S}_2\text{O}_3$.

Section B: Organic Chemistry

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)
2. Separation of mixtures by Chromatography: Measure the R_f value in each case (combination of two compounds to be given)
 - (a) Identify and separate the components of a given mixture of 2 amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by paper chromatography
 - (b) Identify and separate the sugars present in the given mixture by paper chromatography.

Reference Books:

- [1] Vogel's Qualitative Inorganic Analysis, A.I. Vogel, Prentice Hall, 7th Edition.
- [2] Vogel's Quantitative Chemical Analysis, A.I. Vogel, Prentice Hall, 6th Edition.
- [3] Textbook of Practical Organic Chemistry, A.I. Vogel, Prentice Hall, 5th edition.
- [4] Practical Organic Chemistry, F. G. Mann. & B. C. Saunders, Orient Longman, 1960.

CYG-151: Generic Chem.: Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I

(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters)

Section A: Physical Chemistry-1

(30 Lectures)

Chemical Energetics

(10 Lectures)

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.

Chemical Equilibrium:

(8 Lectures)

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

Ionic Equilibria:

(12 Lectures)

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.

Section B: Organic Chemistry-2

(30 Lectures)

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

Aromatic hydrocarbons:

(8 Lectures)

Preparation (Case benzene): from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid.

Reactions: (Case benzene): 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).

Alkyl and Aryl Halides

Alkyl Halides (Upto 5 Carbons): Types of Nucleophilic Substitution (SN_1 , SN_2 and SN_i) 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 $\text{NaNH}_2/\text{NH}_3$).

Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides. (8 Lectures)

Alcohols, Phenols and Ethers (Upto 5 Carbons)

Alcohols:

Preparation: Preparation of 1o, 2o and 3o 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.

Aldehydes and ketones (aliphatic and aromatic): (Formaldehyde, acetaldehyde, acetone and benzaldehyde).

Preparation: from acid chlorides and from nitriles.

Reactions – Reaction with HCN, ROH, NaHSO_3 , $\text{NH}_2\text{-G}$ derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Ponndorf Verley reduction. (14 Lectures)

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

GCL-151: Basic Physical and Organic Chemistry Lab

(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters)

Program:	Integrated M.Sc.	Semester:	Generally chosen at 2 nd Sem
Course Title:	<i>Basic Physical and Organic Chemistry Lab</i>		
Course Code:	<i>GCL-151</i>	Type:	<i>Generic Elective Course</i>
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “ <i>CYG-151: Generic Chem. : Chemical Energetics, Equilibria & Functional Group Org. Chem. I</i> ”		

Section A: Physical Chemistry

Thermochemistry

1. Determination of heat capacity of calorimeter for different volumes.
2. Determination of enthalpy of neutralization of HCl with NaOH.
3. Determination of enthalpy of ionization of acetic acid.
4. Determination of integral enthalpy of solution of salts (KNO₃, NH₄Cl).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of ΔH .

Ionic equilibria

pH measurements

- a) Measurement of 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.
- b) Preparation of buffer solutions: (i) Sodium acetate-acetic acid, and (ii) Ammonium chloride-ammonium hydroxide
Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

Section B: Organic Chemistry

1. Purification of organic compounds by crystallization (from water and alcohol) and distillation.
2. Criteria of Purity: Determination of melting and boiling points.
3. Preparations: Mechanism of various reactions involved to be discussed. Recrystallisation, determination of melting point and calculation of quantitative yields to be done.
 - (a) Bromination of Phenol/Aniline
 - (b) Benzoylation of amines/phenols
 - (c) Oxime and 2,4 dinitrophenylhydrazone of aldehyde/ketone

Reference Books

- [1] A.I. Vogel: Textbook of Practical Organic Chemistry, 5th edition, Prentice-Hall.
- [2] F. G. Mann & B. C. Saunders, Practical Organic Chemistry, Orient Longman (1960).
- [3] B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

CYG-201: Generic Chem.: s- and p-Block Elements, States of Matter and Chemical Kinetics

Section A: Inorganic Chemistry

(30 Lectures)

General Principles of Metallurgy:

(4 Lectures)

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.

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.

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

(26 Lectures)

Section B: Physical Chemistry-3

(30 Lectures)

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. Andrews isotherms of CO_2 .

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).

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)

Solids

Forms of solids. Symmetry elements, unit cells, crystal systems, Bravais lattice types and identification of lattice planes. Laws of Crystallography - Law of constancy of interfacial angles, Law of rational indices. 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.

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).

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.

दून विश्वाविद्यालय
DOON UNIVERSITY
2005

GCL-201: Basic Physical and Inorganic Chemistry Lab

(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters)

Program:	Integrated M.Sc.	Semester:	Generally it is chosen at 3 rd Sem
Course Title:	<i>Basic Physical and Inorganic Chemistry Lab</i>		
Course Code:	<i>GCL-201</i>	Type:	<i>Generic Elective Course</i>
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled " <i>CYG-201: Generic Chem. : s- and p-Block Elements, States of Matter & Chemical Kinetics</i> "		

Section A: Inorganic Chemistry

Semi-micro qualitative analysis using H₂S of mixtures- not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

Cations : NH₄⁺, Pb²⁺, Ag⁺, Bi³⁺, Cu²⁺, Cd²⁺, Sn²⁺, Fe³⁺, Al³⁺, Co²⁺, Cr³⁺, Ni²⁺, Mn²⁺, Zn²⁺, Ba²⁺, Sr²⁺, Ca²⁺, K⁺

Anions : CO₃²⁻, S²⁻, SO₂⁻, S₂O₃²⁻, NO₃⁻, CH₃COO⁻, Cl⁻, Br⁻, I⁻, NO₃⁻, SO₄²⁻, PO₄³⁻, BO₃³⁻, C₂O₄²⁻, F⁻

(Spot tests should be carried out wherever feasible)

Section B: Physical Chemistry

(I) Surface tension measurement (use of organic solvents excluded).

a) Determination of the surface tension of a liquid or a dilute solution using a stalagmometer.

b) Study of the variation of surface tension of a detergent solution with concentration.

(II) Viscosity measurement (use of organic solvents excluded).

a) Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwald's viscometer.

b) Study of the variation of viscosity of an aqueous solution with concentration of solute.

(III) Chemical Kinetics:

Study the kinetics of the following reactions.

(1) Initial rate method: *Iodide-persulphate reaction.*

(2) Integrated rate method: (a) *Acid hydrolysis of methyl acetate with hydrochloric acid,*
(b) *Saponification of ethyl acetate and (c) Compare the strengths of HCl and H₂SO₄ by studying kinetics of hydrolysis of methyl acetate*

Reference Books:

- [1] A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- [2] A.I. Vogel, Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- [3] B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

CYG- 202: Generic Chem.: Chemistry of d-Block Elements, Quantum Chemistry & Spectroscopy

(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters)

Section A: Inorganic Chemistry-3

(30 Lectures)

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).

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.

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.

Section B: Physical Chemistry-4

(30 Lectures)

Quantum Chemistry & Spectroscopy

Spectroscopy and its importance in chemistry. Wave-particle duality. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter. Types of spectroscopy. Difference between atomic and molecular spectra. Born-Oppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components.

Postulates of quantum mechanics, quantum mechanical operators.

Free particle. Particle in a 1-D box (complete solution), quantization, normalization of wavefunctions, concept of zero-point energy.

Rotational Motion: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels.

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.

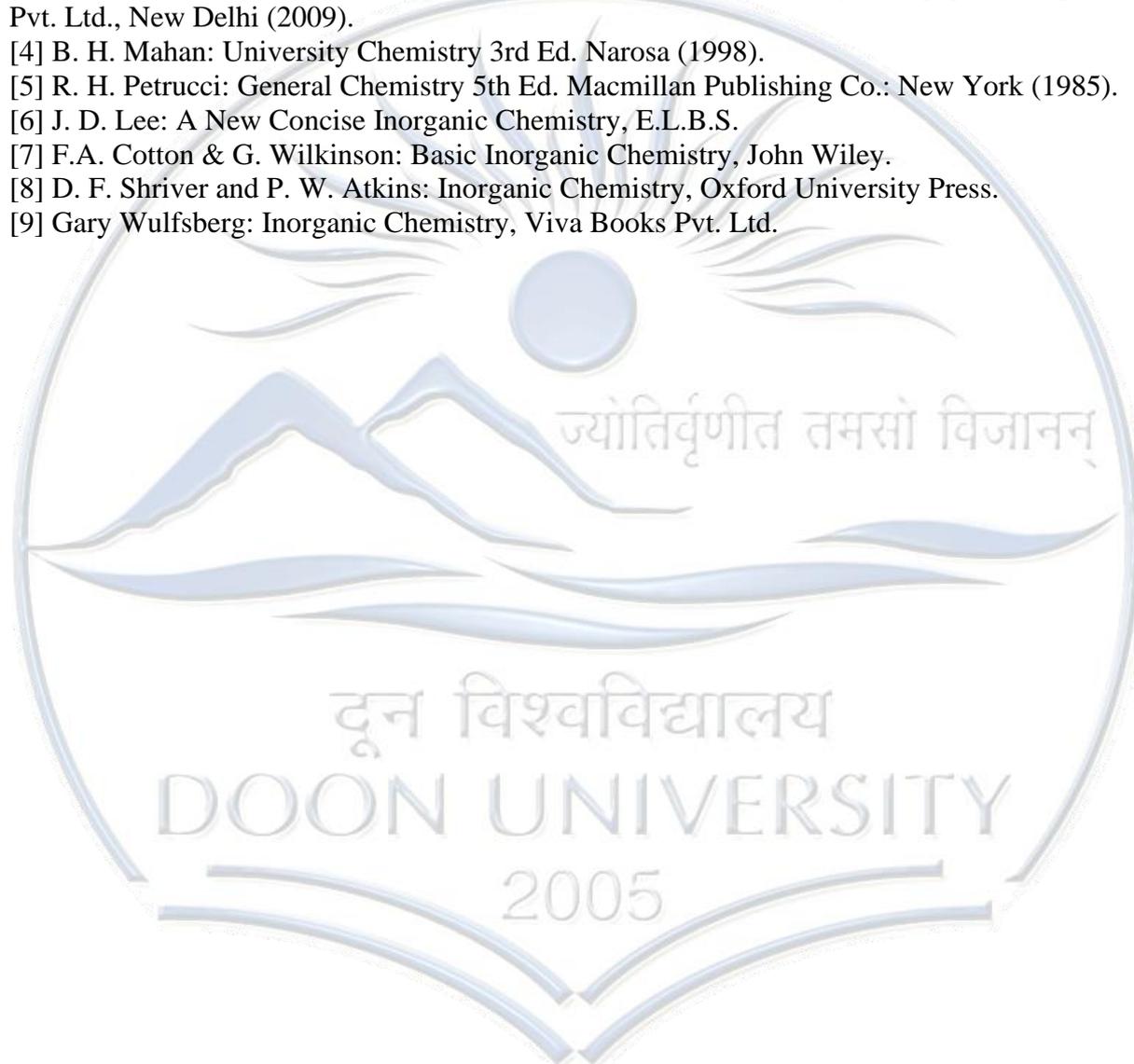
Electronic Spectroscopy: Electronic excited states. Free Electron model and its application to electronic spectra of polyenes. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts.

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. (6 Lectures)

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.



GCL-202: Basic Spectroscopic Analysis Lab

(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters)

Program: Integrated M.Sc.	Semester: Non-Semester Specific
Course Code: GCL-202	Type: Generic Elective Course
Credits: 02	Contact Hours: 04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYG-202: <i>Generic Chem.: Chemistry of d-Block Elements, Quantum Chemistry and Spectroscopy</i> ”

Section A: Inorganic Chemistry

- [1] Estimation of the amount of nickel present in a given solution as bis(dimethylglyoximate) nickel(II) or aluminium as oxinate in a given solution gravimetrically.
- [2] Estimation of (i) Mg^{2+} or (ii) Zn^{2+} by complexometric titrations using EDTA.
- [3] Estimation of total hardness of a given sample of water by complexometric titration.
- [4] 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.
- [5] Determination of the composition of the Fe^{3+} - salicylic acid complex / Fe^{2+} - phenanthroline complex in solution by Job's method.
- [6] Determination of concentration of Na^+ and K^+ using Flame Photometry.

Section B: Physical Chemistry

UV/Visible spectroscopy

- [I] 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).
- [II] Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
- [III] 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.

Colourimetry

- [I] Verify Lambert-Beer's law and determine the concentration of $CuSO_4/KMnO_4/K_2Cr_2O_7$ in a solution of unknown concentration
- [II] 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.

CYG- 203: Generic Chem.: Molecules of Life

(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters. Generally it is offered for or chosen by the students of 3rd Semester)

Unit 1: Carbohydrates

(10 Periods)

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

(12 Periods)

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

(12 Periods)

Mechanism of enzyme action, 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 and Non competitive inhibition including allosteric inhibition). Drug action-receptor theory. Structure –activity relationships of drug molecules, binding role of –OH group, -NH₂ group, double bond and aromatic ring,

Unit 4: Nucleic Acids

(10 Periods)

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

(08 Periods)

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).

Unit 6: Concept of Energy in Biosystems

(8 Periods)

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.

Suggested Readings:

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

Generic Elective Course: 02 Credits

GCL-203: Basic Biochemistry Lab

(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters)

Program: Integrated M.Sc.	Semester: Commonly offered at 3 rd Semester
Course Code: GCL-203	Type: Generic Elective Course
Credits: 02	Contact Hours: 04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYG-203: <i>Generic Chem.: Molecules of Life</i> ”

- [1] Separation of amino acids by paper chromatography
- [2] To determine the concentration of glycine solution by formylation method.
- [3] Study of titration curve of glycine
- [4] Action of salivary amylase on starch
- [5] 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] Differentiate between a reducing/ nonreducing sugar.
- [9] Extraction of 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] Furniss, B.S.; Hannaford, A.J.; Rogers, V.; Smith, P.W.G.; Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, ELBS.
- [2] Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry, Universities Press.

DOON UNIVERSITY
2005

CYG-252: Generic Chem.: Organometallics, Bioinorganic Chemistry, Polymer Hydrocarbons and UV-IR Spectroscopy

(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters)

Section A: Inorganic Chemistry-4

(30 Lectures)

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, $[Co(NH_3)_6]Cl_3$, $Na_3[Co(NO_2)_6]$. (6 Lectures)

Organometallic Compounds

Definition and Classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p and multicentre bonds). Structures of methyl lithium, Zeiss salt and ferrocene. EAN rule as applied to carbonyls. Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d metals. π -acceptor behaviour of carbon monoxide. Synergic effects (VB approach)- (MO diagram of CO can be referred to for synergic effect to IR frequencies). (12 Lectures)

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). (12 Lectures)

Section B: Organic Chemistry-4

(30 Lectures)

Polynuclear and heteronuclear aromatic compounds:

Properties of the following compounds with reference to electrophilic and nucleophilic substitution: Naphthalene, Anthracene, Furan, Pyrrole, Thiophene, and Pyridine. (6 Lectures)

Active methylene compounds:

Preparation: Claisen ester condensation. Keto-enol tautomerism.

Reactions: Synthetic uses of ethylacetoacetate (preparation of non-heteromolecules having upto 6 carbon). (6 Lectures)

Application of Spectroscopy to Simple Organic Molecules

Application of visible, ultraviolet and Infrared spectroscopy in organic molecules. Electromagnetic radiations, electronic transitions, λ_{max} and ϵ_{max} , chromophore, auxochrome, bathochromic and hypsochromic shifts. Application of electronic spectroscopy and Woodward rules for calculating λ_{max} of conjugated dienes and α, β – unsaturated compounds. Infrared radiation and types of molecular vibrations, functional group and fingerprint region. IR spectra of alkanes, alkenes and simple alcohols (inter and intramolecular hydrogen bonding), aldehydes, ketones, carboxylic acids and their derivatives (effect of substitution on $>C=O$ stretching absorptions). (18 Lectures)

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.

GCL-252: Inorg. and Org. Synthesis and Qualitative Analysis Lab

(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters)

Program:	Integrated M.Sc.	Semester:	Commonly offered at 4 th Semester
Course Title:	<i>Inorg. & Org. Synthesis and Qualitative Analysis Lab</i>		
Course Code:	<i>GCL-252</i>	Type:	<i>Generic Elective Course</i>
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “ <i>CYG-252: Generic Chem. : Organometallics, Bioinorganic Chemistry, Polynuclear Hydrocarbons and UV-IR Spectroscopy</i> ”		

Section A: Inorganic Chemistry

- [1] Separation of mixtures by chromatography: Measure the *R_f* value in each case (Combination of two ions to be given).
Paper chromatographic separation of Fe³⁺, Al³⁺ and Cr³⁺ or
Paper chromatographic separation of Ni²⁺, Co²⁺, Mn²⁺ and Zn²⁺
- [2] Preparation of 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, MgCl₂ and LiCl₃.*

Section B: Organic Chemistry

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] A.I. Vogel: Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- [2] A.I. Vogel: Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- [3] A.I. Vogel: Textbook of Practical Organic Chemistry, Prentice Hall, 5th Edn.
- [4] F. G. Mann & B. C. Saunders: Practical Organic Chemistry, Orient Longman (1960).

CYG- : Generic Chem.: Solutions, Phase Equilibrium, Conductance, Electrochemistry & Functional Group Organic Chemistry-II

(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters)

Section A: Physical Chemistry-2

(30 Lectures)

Solutions

Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, deviations from Raoult's law – non-ideal solutions. Vapour pressure-composition and temperature-composition curves of ideal and non-ideal solutions. Distillation of solutions. Lever rule. Azeotropes.

Partial miscibility of liquids: Critical solution temperature; effect of impurity on partial miscibility of liquids. Immiscibility of liquids- Principle of steam distillation. Nernst distribution law and its applications, solvent extraction.

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 83 sulphur) and two component systems involving eutectics, congruent and incongruent melting points (lead-silver, $\text{FeCl}_3\text{-H}_2\text{O}$ and Na-K only).

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).

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).

Section B: Organic Chemistry-3

(30 Lectures)

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

Carboxylic acids and their derivatives:

Carboxylic acids (aliphatic and aromatic):

Preparation: Acidic and Alkaline hydrolysis of esters.

Reactions: Hell – Vohlard - Zelinsky Reaction.

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.

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.

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 $-\text{COOH}$ group, acetylation of $-\text{NH}_2$ 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.

Carbohydrates:

Classification, and General Properties, Glucose and Fructose (open chain and cyclic structure), Determination of configuration of monosaccharides, absolute configuration of Glucose and Fructose, Mutarotation, ascending and descending in monosaccharides. Structure of disaccharides (sucrose, cellobiose, maltose, lactose) and polysaccharides (starch and cellulose) excluding their structure elucidation.

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] Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

[7] Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Phase Equilibria, Electrochemistry and Qualitative Org. Analysis Lab

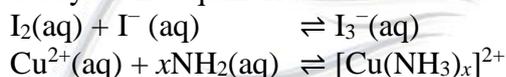
(Non-Semester Specific and for the Students of First, Second, Third or Fourth Semesters)

Program: Integrated M.Sc.	Semester: Non-Semester Specific
Course Code: GCL-.....	Type: Generic Elective Course
Credits: 02	Contact Hours: 04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled "CYG-.....: <i>Generic Chem.: Solutions, Phase Equilibrium, Conductance, Electrochemistry & Functional Group Organic Chemistry-II</i>

Section A: Physical Chemistry

Distribution

Study of the equilibrium of one of the following reactions by the distribution method:



Phase equilibria

- [a] Construction of the phase diagram of a binary system (simple eutectic) using cooling curves.
- [b] Determination of the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.
- [c] Study of the variation of mutual solubility temperature with concentration for the phenol water system and determination of the critical solubility temperature.

Conductance

- [d] Determination of cell constant
- [e] Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
- [f] Perform the following conductometric titrations:
 - (i) Strong acid vs. strong base
 - (ii) Weak acid vs. strong base

Potentiometry

Perform the following potentiometric titrations:

- [g] Strong acid vs. strong base
- [h] Weak acid vs. strong base
- [i] Potassium dichromate vs. Mohr's salt

Section B: Organic Chemistry

[I] Systematic Qualitative Organic Analysis of Organic Compounds possessing monofunctional groups (-COOH, phenolic, aldehydic, ketonic, amide, nitro, amines) and preparation of one derivative.

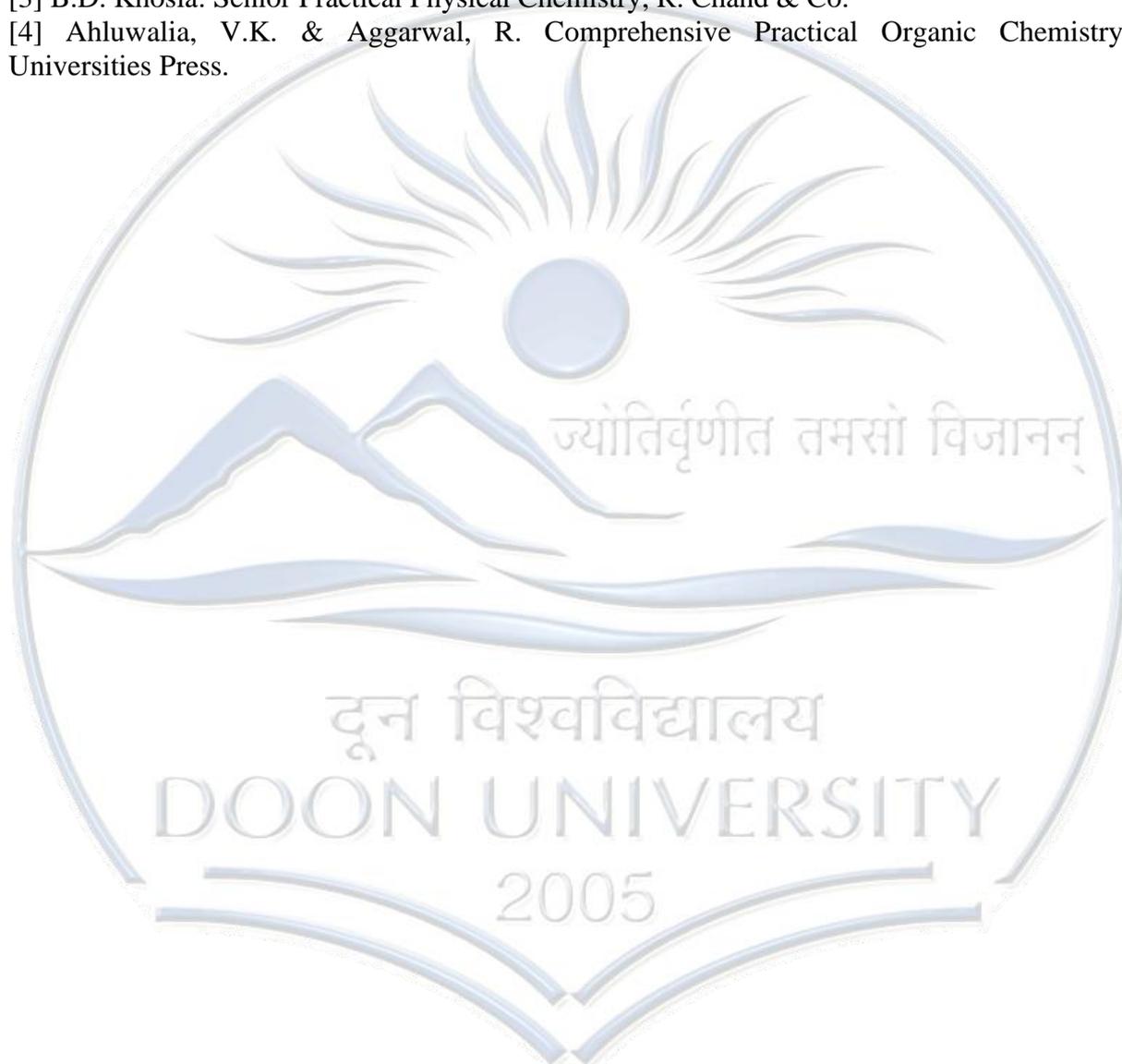
[II]

- [1] Separation of amino acids by paper chromatography
- [2] Determination of the concentration of glycine solution by formylation method.
- [3] Titration curve of glycine

- [4] Action of salivary amylase on starch
- [5] Effect of temperature on the action of salivary amylase on starch.
- [6] Determination of the saponification value of an oil/fat.
- [7] Determination of the iodine value of an oil/fat
- [8] Differentiation between a reducing/nonreducing sugar.
- [9] Extraction of DNA from onion/ cauliflower

Reference Books:

- [1] A.I. Vogel: Textbook of Practical Organic Chemistry, Prentice Hall, 5th Edn.
- [2] F. G. Mann & B. C. Saunders: Practical Organic Chemistry, Orient Longman, 1960.
- [3] B.D. Khosla: Senior Practical Physical Chemistry, R. Chand & Co.
- [4] Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry, Universities Press.



Skill Enhancement Course
CYS-201: Fuel Chemistry
(Non-Semester Specific and for the students of 3rd or 4th Semester)

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.

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.

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.

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-251: Pesticide Chemistry
(Non-Semester Specific and for the students of 3rd or 4th Semester)

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).

Practicals:

- [1] To calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
- [2] Preparation of simple organophosphates, phosphonates and thiophosphates

Suggested Readings:

- [1] R. Cremlyn: Pesticides, John Wiley

Skill Enhancement Course
CYS-255: Chemistry of Cosmetics and Perfumes
(Non-Semester Specific and for the students of 3rd or 4th Semester)

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.

Practicals

- [1] Preparation of talcum powder.
- [2] Preparation of shampoo.
- [3] Preparation of enamels.
- [4] Preparation of hair remover.
- [5] Preparation of face cream.
- [6] Preparation of 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-: IT Skills for Chemists

(Non-Semester Specific and for the students of 3rd or 4th Semester)

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).

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).

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
Chemical Technology and Society
(Non-Semester Specific and for the students of 3rd or 4th Semester)

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.

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.

ज्योतिर्वृणीत तमसो विजानन्

Skill Enhancement Course

Business Skills for Chemists

(Non-Semester Specific and for the students of 3rd or 4th Semester)

Business Basics

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

Chemistry in Industry

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

Making money

Financial aspects of business with case studies

Intellectual property

Concept of intellectual property, patents.

Reference:

www.rsc.org

Skill Enhancement Course
Cheminformatics
(Non-Semester Specific and for the students of 3rd or 4th Semester)

Introduction to Chemoinformatics:

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

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.

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.

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

दून विश्वाविद्यालय
DOON UNIVERSITY
2005

Skill Enhancement Course
Intellectual Property Rights (IPR)
(Non-Semester Specific and for the students of 3rd or 4th Semester)

Introduction to Intellectual Property:

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

Copyrights:

Introduction, How to obtain, Differences from Patents.

Trade Marks:

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, Trade names, etc.

Differences from Designs.

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.

Geographical Indications:

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Industrial Designs:

Definition, How to obtain, features, International design registration.

Layout design of integrated circuits:

Circuit Boards, Integrated Chips, Importance for electronic industry.

Trade Secrets:

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

Different International Agreements:

(a) World 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

WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity

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
Analytical Clinical Biochemistry
(Non-Semester Specific and for the students of 3rd or 4th Semester)

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 polysaccharides.

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.

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.

Practicals:

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; G. P. Talwar and M. Srivastava: Textbook of Biochemistry and Human Biology; and A.L. Lehninger: Biochemistry.
- [2] Keith Wilson and John Walker: Practical Biochemistry. • Alan H Gowenlock: Varley’s Practical Clinical Biochemistry.

Skill Enhancement Course
Green Methods in Chemistry
(Non-Semester Specific and for the students of 3rd or 4th Semester)

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 CO₂ for precision cleaning and dry cleaning of garments.
- [3] Environmentally safe antifoulant.
- [4] CO₂ 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

Skill Enhancement Course
Pharmaceutical Chemistry
(Non-Semester Specific and for the students of 3rd or 4th Semester)

Drugs & Pharmaceuticals

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, Ibuprofen); 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).

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.

Practicals

- [1] Preparation of Aspirin and its analysis.
- [2] Preparation of magnesium bisilicate (Antacid).

Suggested Readings:

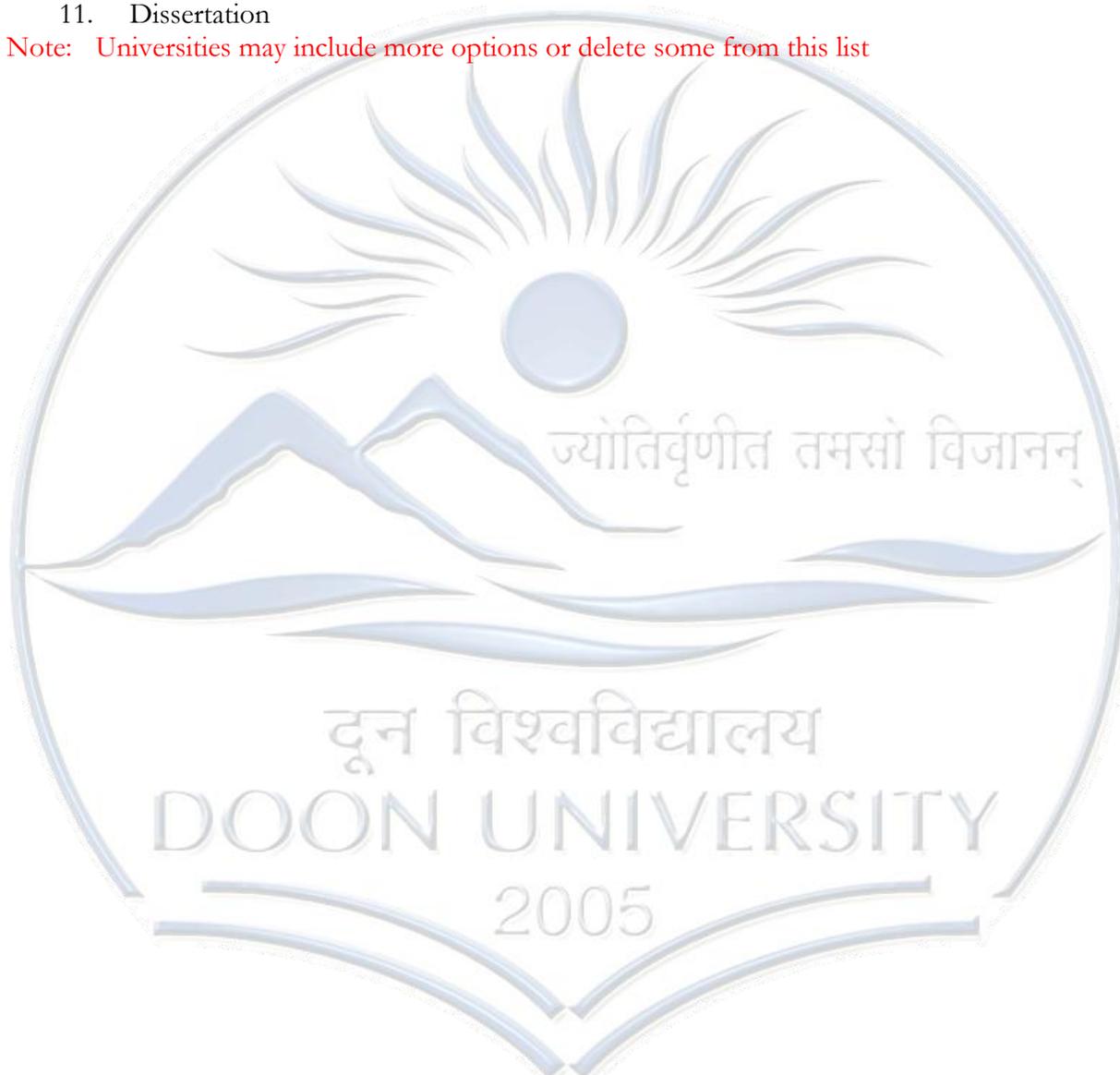
- [1] G.L. Patrick: Introduction to Medicinal Chemistry, Oxford University Press, UK.
- [2] Hakishan, V.K. Kapoor: Medicinal and Pharmaceutical Chemistry, Vallabh Prakashan, Pitampura, New Delhi.
- [3] William O. Foye, Thomas L., Lemke, David A. William: Principles of Medicinal Chemistry, B.I. Waverly Pvt. Ltd. New Delhi.

Discipline Specific Elective Courses: (Credit: 06 each)

(Students opt any 4 papers from the following list in the 3rd Year of Integrated M.Sc. Program)

- | | |
|---|--------------------------------------|
| 1. Polymer Chemistry | (04 Credits) + Lab (02 Credits) |
| 2. Inorganic Materials of Industrial Importance | (04 Credits) + Lab (02 Credits) |
| 3. Novel Inorganic Solids | (04 Credits) + Lab (02 Credits) |
| 4. Research Methodology for Chemistry | (05 Credits) + Tutorials (01 Credit) |
| 5. Applications of Computers in Chemistry | (04 Credits) + Lab (02 Credits) |
| 6. Molecular Modelling & Drug Design | (04 Credits) + Lab (02 Credits) |
| 7. Industrial Chemicals & Environment | (04 Credits) + Lab (02 Credits) |
| 11. Dissertation | |

Note: Universities may include more options or delete some from this list



**CYD-302: Discipline Specific Elective:
Polymer Chemistry**

(Non-Semester Specific and for the Students of 5th or 6th Semester)

Introduction and History of Polymeric Materials:

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers.

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.

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.

Crystallization and Crystallinity:

Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.

Nature and Structure of Polymers:

Structure Property relationships.

Determination of Molecular Weight of Polymers (M_n , M_w , etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance.

Polydispersity index.

Glass Transition Temperature (T_g) and Determination of T_g , Free volume theory, WLF equation, Factors affecting glass transition temperature (T_g).

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.

Properties of Polymers (Physical, thermal, Flow & Mechanical Properties).

Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes,

Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide polypyrrole, polythiophene)].

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. • R.W. Lenz: Organic Chemistry of Synthetic High Polymers.

Discipline Specific Elective Course: 02 Credits

DCL-302: Polymer Chemistry Lab

(Non-Semester Specific and for the Students of 5th or 6th Semester)

Program:	Integrated M.Sc.	Semester:	Non-Semester Specific
Course Title:	<i>Polymer Chemistry Lab</i>		
Course Code:	DCL-302	Type:	Discipline Specific Elective
Credits:	02	Contact Hours:	04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYD-302: <i>Discipline Specific Elective: Polymer Chemistry</i> ”		

[A] Polymer Synthesis

- (1) Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).
 - a. Purification of monomer
 - b. Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bis-isobutyronitrile (AIBN)
- (2) Preparation of nylon 66/6
 1. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein
 - a. Preparation of IPC
 - b. Purification of IPC
 - c. Interfacial polymerization
- (3) Redox polymerization of acrylamide
- (4) Precipitation polymerization of acrylonitrile
- (5) Preparation of urea-formaldehyde resin
- (6) Preparations of novalac resin/resold resin.
- (7) Microscale Emulsion Polymerization of Poly(methylacrylate).

[B] Polymer Characterization

- (1) Determination of molecular weight by viscometry:
 - (a) Polyacrylamide-aq. NaNO₂ solution, (b) (Poly vinyl propylidene (PVP) in water
- (2) Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of “head-to-head” monomer linkages in the polymer.
- (3) Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).
- (4) Testing of mechanical properties of polymers.
- (5) Determination of hydroxyl number of a polymer using colorimetric method.

[C] Polymer Analysis

- (1) Estimation of the amount of HCHO in the given solution by sodium sulphite method
- (2) Instrumental Techniques
- (3) IR studies of polymers
- (4) DSC analysis of polymers
- (5) Preparation of polyacrylamide and its electrophoresis

*at least 7 experiments to be carried out.

Suggested Readings:

- [1] Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
- [2] Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003).
- [3] Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
- [4] Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)

CYD-303: Discipline Specific Elective: Inorganic Materials of Industrial Importance

(Non-Semester Specific and for the Students of 5th or 6th Semester)

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.

Fertilizers:

Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

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.

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.

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.

Catalysis:

General principles and properties of catalysts, homogenous catalysis (catalytic steps and examples) and heterogenous catalysis (catalytic steps and examples) and their industrial applications, Deactivation or regeneration of catalysts.

Phase transfer catalysts, application of zeolites as catalysts.

Chemical explosives:

Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants.

Suggested Readings: [1] E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK; B. K. Sharma: *Engineering Chemistry*, Goel Publishing House, Meerut.

Discipline Specific Elective Course: 02 Credits

CYD-303: Industrial Inorganic Materials Lab

(Non-Semester Specific and for the Students of 5th or 6th Semester)

Program: Integrated M.Sc. **Semester:** Non Semester Specific
Course Title: *Industrial Inorganic Materials Lab*
Course Code: DCL-303 **Type:** Discipline Specific Elective
Credits: 02 **Contact Hours:** 04 × 15 (04 Hr/Week)
Corresponding Theory Course: To be offered in combination with the theory course titled “CYD-303: *Discipline Specific Elective: Inorganic Materials of Industrial Importance*”

1. Determination of free acidity in ammonium sulphate fertilizer.
2. Estimation of Calcium in Calcium ammonium nitrate fertilizer.
3. Estimation of phosphoric acid in superphosphate fertilizer.
4. Electroless metallic coatings on ceramic and plastic material.
5. Determination of composition of dolomite (by complexometric titration).
6. Analysis of (Cu, Ni); (Cu, Zn) in alloy or synthetic samples.
7. Analysis of Cement.
8. Preparation of pigment (zinc oxide).

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] W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
- [4] J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
- [5] P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
- [6] R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
- [7] B. K. Sharma: *Engineering Chemistry*, Goel Publishing House, Meerut

Discipline Specific Elective Course: 04 Credits

CYD-304: Discipline Specific Elective: Novel Inorganic Solids

(Non-Semester Specific and for the Students of 5th or 6th Semester)

Synthesis and Modification of Inorganic Solids:

Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods.

Inorganic Solids of Technological Importance:

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments.

Molecular material and fullerenes, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

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. Bio-inorganic nanomaterials, DNA and nanomaterials, natural and artificial nanomaterials, bionano composites.

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, copper, aluminum and their alloys like duralumin, brasses and bronzes cutting tool materials, super alloys thermoplastics, thermosets and composite materials.

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.

Speciality Polymers:

Conducting polymers - Introduction, conduction mechanism, polyacetylene, polyparaphenylene and polypyrrole, applications of conducting polymers, Ion-exchange resins and their applications. Ceramic & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications.

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.

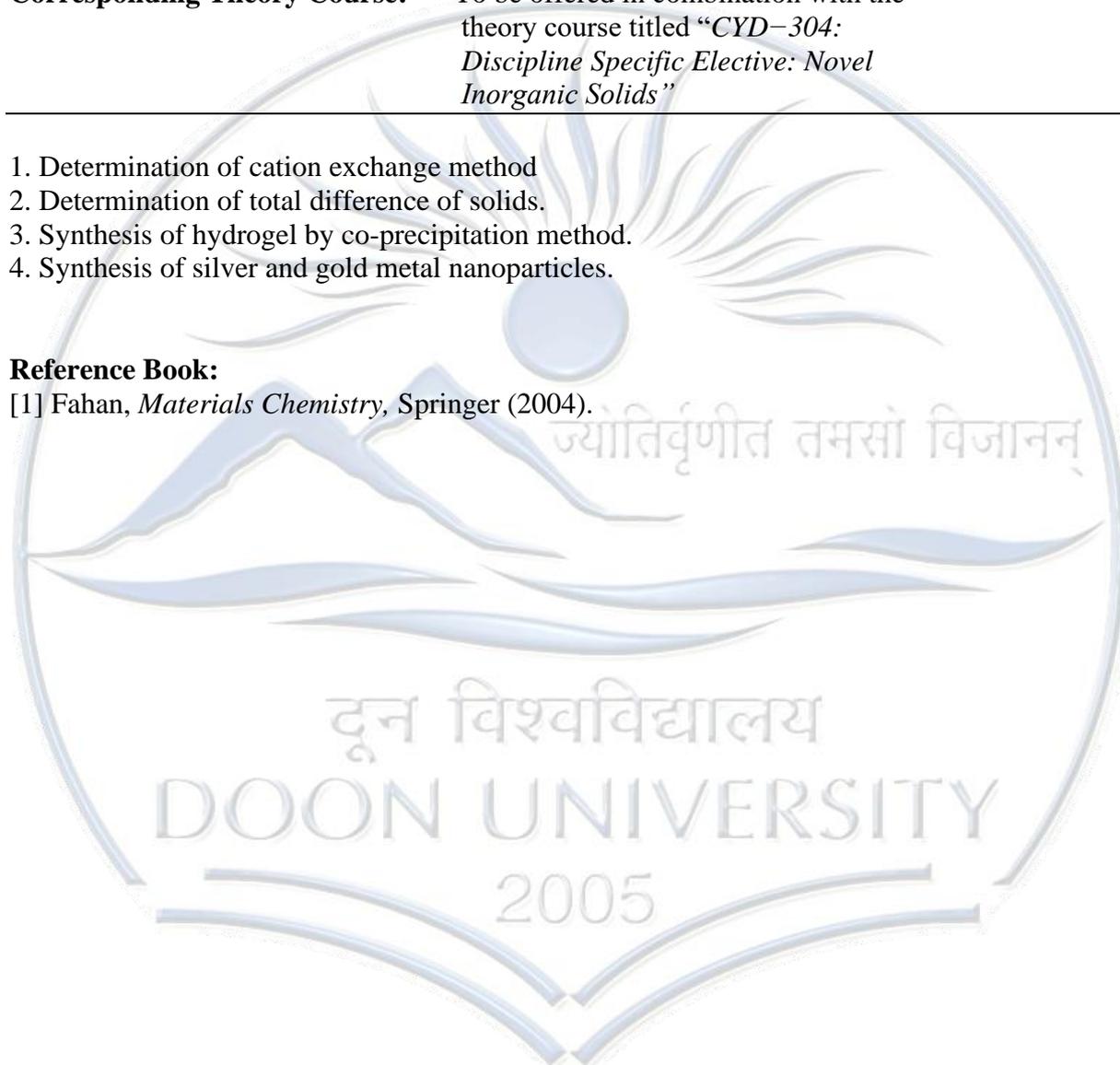
Discipline Specific Elective Course: 02 Credits
DCL-304: Materials Chemistry Lab
(Non-Semester Specific and for the Students of 5th or 6th Semester)

Program: Integrated M.Sc. **Semester:** Non Semester Specific
Course Title: *Materials Chemistry Lab*
Course Code: DCL-304 **Type:** Discipline Specific Elective
Credits: 02 **Contact Hours:** 04 × 15 (04 Hr/Week)
Corresponding Theory Course: To be offered in combination with the theory course titled “CYD-304: *Discipline Specific Elective: Novel Inorganic Solids*”

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.

Reference Book:

[1] Fahan, *Materials Chemistry*, Springer (2004).



Discipline Specific Elective Course: 06 Credits
CYD-352: Discipline Specific Elective:
Research Methodology for Chemistry
(Non-Semester Specific and for the Students of 5th or 6th Semester)

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.

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.

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.

Data Analysis:

The Investigative Approach: Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments.

Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, r and its abuse. Basic aspects of multiple linear regression analysis.

Electronics:

Basic fundamentals of electronic circuits and their components used in circuits of common instruments like spectrophotometers, typical circuits involving operational amplifiers for electrochemical instruments. Elementary aspects of digital electronics.

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

CYD-305: Discipline Specific Elective:
Applications of Computers in Chemistry
(Non-Semester Specific and for the Students of 5th or 6th Semester)

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.

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.

Lab:

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 change 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).

Discipline Specific Elective Course: 02 Credits
DCL-305: Computational Chemistry Lab
(Non-Semester Specific and for the Students of 5th or 6th Semester)

Program: Integrated M.Sc.	Semester: Non Semester Specific
Course Title: <i>Computational Chemistry Lab</i>	
Course Code: DCL-305	Type: Discipline Specific Elective
Credits: 02	Contact Hours: 04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYD-305: <i>Discipline Specific Elective: Applications of Computers in Chemistry</i> ”

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 change 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] McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
- [2] Mortimer, R. *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier (2005).
- [3] Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
- [4] Yates, P. *Chemical Calculations*. 2nd 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).

CYD-306: Molecular Modelling and Drug Design

(Non-Semester Specific and for the Students of 5th or 6th Semester)

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.

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.

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.

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.

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.

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

Discipline Specific Elective Course: 02 Credits
DCL-306: Molecular Modelling Lab
(Non-Semester Specific and for the Students of 5th or 6th Semester)

Program: Integrated M.Sc. **Semester:** Non Semester Specific
Course Title: *Molecular Modelling Lab*
Course Code: DCL-306 **Type:** Discipline Specific Elective
Credits: 02 **Contact Hours:** 04 × 15 (04 Hr/Week)
Corresponding Theory Course: To be offered in combination with the theory course titled “CYD-306: *Discipline Specific Elective: Molecular Modelling and Drug Design*”

- [1] 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) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.
- [3] 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) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- [5] (a) 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) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- [6] 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) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- [8] 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) Compare the optimized bond angles H₂O, H₂S, H₂Se. (b) 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.

Reference Books:

- [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.

Discipline Specific Elective Course: 04 Credits
CYD-351: Discipline Specific Elective:
Industrial Chemicals & Environment
(Non-Semester Specific and for the Students of 5th or 6th Semester)

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.

Industrial Metallurgy

Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconductor technology.

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 SO₂, CO₂, CO, NO_x, H₂S 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.

Energy & Environment

Sources of Energy: Coal, petrol and natural gas. Nuclear Fusion / Fission, Solar energy, Hydrogen, geothermal, Tidal and Hydel, etc.

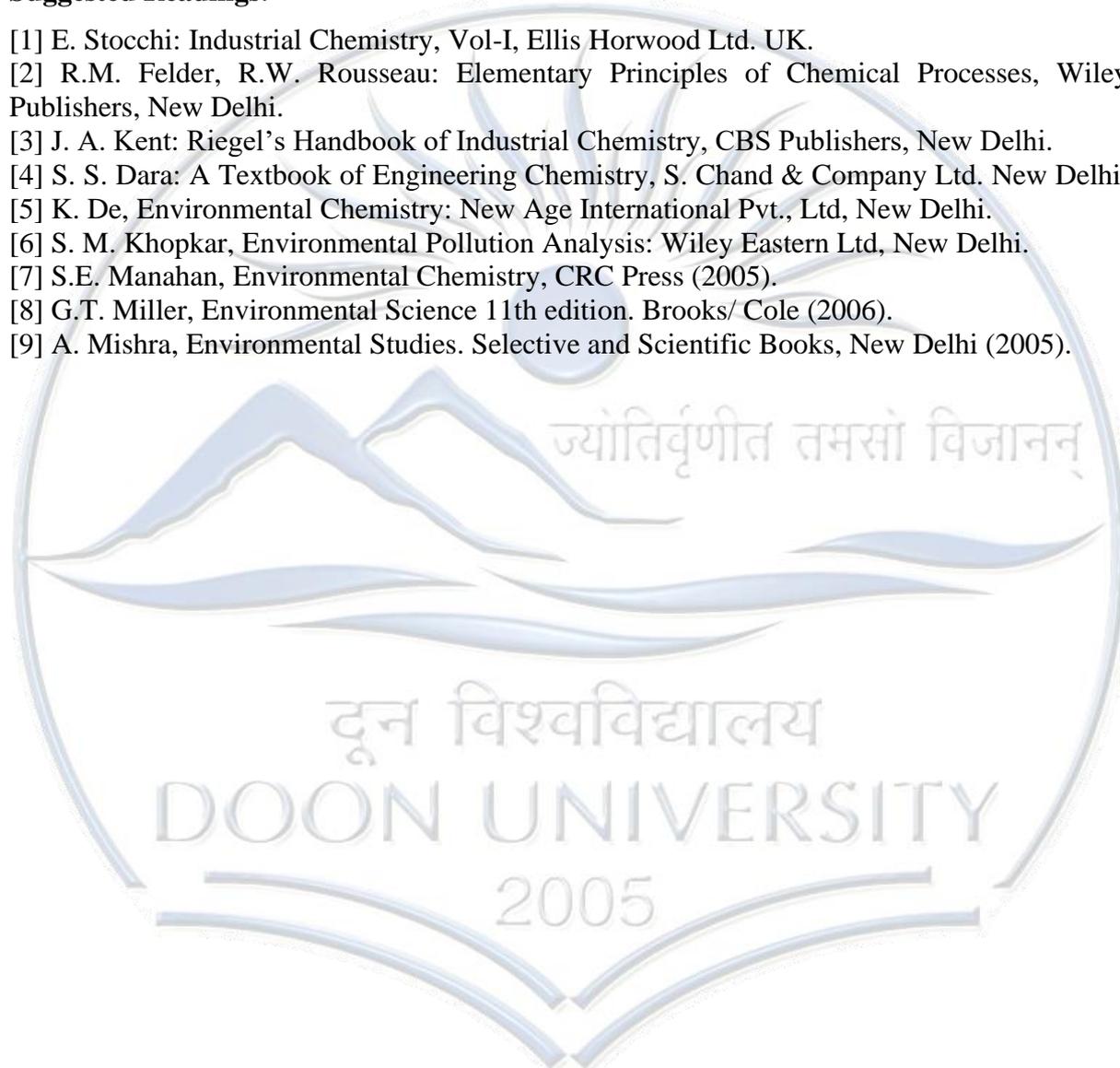
Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management.

Biocatalysis

Introduction to biocatalysis: Importance in “Green Chemistry” and Chemical Industry.

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).



DCL-351: Environmental and Industrial Chemistry Lab

(Non-Semester Specific and for the Students of 5th or 6th Semester)

Program: Integrated M.Sc.	Semester: Non Semester Specific
Course Title: <i>Environmental and Industrial Chemistry Lab</i>	
Course Code: DCL-351	Type: Discipline Specific Elective
Credits: 02	Contact Hours: 04 × 15 (04 Hr/Week)
Corresponding Theory Course:	To be offered in combination with the theory course titled “CYD-351: <i>Discipline Specific Elective: Industrial Chemicals and Environment</i> ”

- [1] Determination of dissolved oxygen in water.
- [2] Determination of Chemical Oxygen Demand (COD)
- [3] Determination of Biological Oxygen Demand (BOD)
- [4] Percentage of available chlorine in bleaching powder.
- [5] Measurement of chloride, sulphate and salinity of water samples by simple titration method (AgNO₃ and potassium chromate).
- [6] Estimation of total alkalinity of water samples (CO₃²⁻, HCO₃⁻) using double titration method.
- [7] Measurement of dissolved CO₂.
- [8] Study of some of the common bio-indicators of pollution.
- [9] Estimation of SPM in air samples.
- [10] Preparation of 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.

CYC-401: Structure and Reactivity of Organic Molecules

(Core Course: 03 Credits and 45 contact hours)

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.

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.

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 (σ), reaction constant (ρ), 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.

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.

7th Semester of Integrated M.Sc.

or

1st Semester of 02 Year-M.Sc.

CYC-402: Thermodynamics and Interfaces

(Core Course: 03 Credits and 45 contact hours)

Unit 1: Classical Thermodynamics

Thermodynamic treatment of phase equilibria, thermodynamic properties of solutions, chemical potential, chemical potential of real gases and fugacity, thermodynamic function of mixing, thermodynamic treatment of ideal and non-ideal solutions, concept of activity, excess thermodynamic functions. Thermodynamic equilibria in one and two component systems.

Unit 2: 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 3: 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.

Unit 4: 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.

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.

7th Semester of Integrated M.Sc.

or

1st Semester of 02 Year-M.Sc.

CYC-403: Solid State Chemistry

(Core Course: 03 Credits and 45 contact hours)

Unit 1: 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 2: 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 3: 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 4: 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 5: 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 Semester of Integrated M.Sc.

or

1st Semester of 02 Year-M.Sc.

CYC-404: Structure and Properties of Metal Complexes

(Core Course: 03 Credits and 45 contact hours)

Unit I: Stereochemistry and bonding in main group compounds

VSEPR theory, Walsh diagrams (tri- and penta-atomic molecules) d_r - p_r 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 and spectrophotometry.

Unit IV: Electronic spectra of coordination compounds:

Spectroscopic ground states, correlation and spin-orbit coupling in free ions for 1st series of transition metals, Orgel and Tanabe Sugano diagrams for transition metal complexes (dⁿ-dⁿ 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 momentum 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**.

CYC-405: Instrumental Methods of Analysis-I

(Core Course: 03 Credits)

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: 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), Electrophoresis (plates and capillary) and use with DNA analysis.

Immunoassays and DNA techniques

Unit III: 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-, Portable IR instrument- and rapid detection.

UV-Visible/ Near IR - Emission, Absorption, Fluorescence and Photoacoustic. 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 IV: 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 V: Electroanalytical Methods: Potentiometry & Voltammetry (dependence on technique), Detection of radiation

Unit VI: 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 Semester of Integrated M.Sc.

or

1st Semester of 02 Year-M.Sc.

CYC-406: Inorganic Chemistry Lab-I

(Core Course: 02 Credits and 60 Contact Hours)

- [1] Semi-micro qualitative analysis involving 6 radicals including interfering radicals.
- [2] Determination of hardness of water by complexometric titration with EDTA.
- [3] Gravimetric estimation of nickel using dimethyl glyoxime.
- [4] Determination of metal ions by gravimetric-cum-volumetric analysis: Fe(II) gravimetrically and Ca(II) volumetrically.
- [5] Determination of Cu(II) gravimetrically and Zn(II) volumetrically
- [6] Experiment related to gravimetric determination and separation of two metal ions in a binary mixture.
- [7] Synthesis of following coordination compound(s) and metal content determination:
(i) $[\text{Cu}(\text{NH}_3)_4\text{H}_2\text{O}]\text{SO}_4$, (ii) $[\text{Fe}(\text{acac})_3]$, (iii) $[\text{Mn}(\text{acac})_3]$, (iv) $\text{Mn C}_2\text{O}_4 \cdot 3\text{H}_2\text{O}$.

Note: Minimum five experiments must be done and some experiments would require more than one turn

Suggested Readings

- [1] Mendham, J., Denney, R.C., Barnes J.D. and Thomas M.J., "Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed., ELBS Longman Group UK Ltd. (2004)
- [2] Vogel's *Qualitative Inorganic Analysis*, Revised by G. Svehla. Marr & Rockett "Inorganic Preparations"
- [3] Srivastava T.N. and Kamboj P.C., "Analytical Chemistry", Vishal Publications.
- [4] Marr & Rockett "Practical Inorganic Chemistry"

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2005

7th Semester of Integrated M.Sc.

or

1st Semester of 02 Year-M.Sc.

CYC-407: Organic Chemistry Lab-I

(Core Course: 02 Credits and 60 Contact Hours)

- [1] Separation of organic mixtures by TLC and PTLC.
- [2] Synthesis of derivatives for carbonyl, amino and active methylene compounds.
- [3] Diels-Alder reaction between anthracene and maleic anhydride.
- [4] Oxidation of hydroquinone to p-benzoquinone.
- [5] Oxidation of benzoin to benzyl.
- [6] Conversion of benzyl to quinoxaline.
- [7] Reduction of Camphor.
- [8] Aldol condensation (benzaldehyde + acetone or cinnamaldehyde + acetone)
- [9] Synthesis of 2-iodobenzoic acid by Sandmeyer reaction.
- [10] Synthesis of binaphthol by green reaction.
- [11] Knoevenagel condensation between aldehyde (4-diethylaminobenzaldehyde) and malonic acid, cyanoacetic acid or malononitrile.
- [12] Friedel-Crafts reaction: synthesis of 1,4-di-tert-butyl-2,5-dimethoxy benzene.
- [13] Preparation and purification of cis- and trans-stilbenes by Wittig reaction.
- [14] Bromination of acetanilide.

Note: Minimum five experiments must be done and some would require more two-three turns.

Suggested Readings

- [1] Arthur, I. V. *Quantitative Organic Analysis*, Pearson.
- [2] Furniss B.S., Hannaford A.J., Smith P.W.G. and Tatchell A.R., "*Vogel's Text Book of Practical Organic Chemistry*", 5th Ed., Longman.
- [3] Leonard J., Lygo B. and Procter G., "*Advanced Practical Organic Chemistry*", Chapman & Hall.
- [4] Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education.
- [5] Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, 5th Ed., Pearson

7th Semester of Integrated M.Sc.

or

1st Semester of 02 Year-M.Sc.

CYC-408: Physical Chemistry Lab-I

(Core Course: 02 Credits and 60 Contact Hours)

- [1] To study the variation in miscibility of phenol in water with temperature and to find out the critical solution temperature (CST) and also to investigate the effect of impurities on CST.
- [2] To determine the cell potentials for different electrochemical cells and also to measure different thermodynamic parameters.
- [3] Verification of Freundlich's adsorption isotherms and calculation of characteristic constants.
- [4] Verification of Langmuir adsorption isotherms and determination of surface area.
- [5] Rate of Hydrolysis of Sucrose using polarimeter.
- [6] Determination of isotherm for three component system.
- [7] To determine the magnetic susceptibility of solids.
- [8] To determine refractive index of dielectric layer using SPR

Note: Minimum five experiments must be done and some would require more two-three turns.

Suggested Readings

- [1] Levitt, B.P., "*Findlay's Practical Physical Chemistry*", 9th Ed., Longman Garland C.W.,
- [2] Nifler J.W. and Schoemaker D.P., "*Experiments in Physical Chemistry*", 7th Ed., JMCGra,-Hill International.
- [3] Halpern, A. M. & McBane, G. C., "*Experimental Physical Chemistry 3rd Ed.*"; W.H. Freeman & Co.: New York

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DOON UNIVERSITY
2005

CYC-451: Pericyclic and Organic Photochemistry

(Core Course: 03 Credits)

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 suprafacial addition, $4n$ and $4n+2$ systems, 2+2 addition of ketenes, 1,3 dipolar cycloaddition, Diels-Alder Reaction and its variants, Cheletropic 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. Paterno-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. Ramamurthy & J. C. Scaiano, "*Modern molecular photochemistry of organic Compounds*", University Science Books (2010).

8th Semester of Integrated M.Sc.

or

2nd Semester of 02 Year-M.Sc.

CYC-452: Reagents and Reactions in Organic Chemistry

(Core Course: 03 Credits)

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 Umpolung), 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 enamines, enolates, lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates, mechanism of aldol (Mukaiyama 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", 3^s Ed., Academic Press.
- [5] Bruckner, R., "Organic Mechanisms: Reactions, Stereochemistry and Synthesis", Springer.

8th Semester of Integrated M.Sc.

or

2nd Semester of 02 Year-M.Sc.

CYC-453: Kinetics and Photochemistry

(Core Course: 03 Credits)

Unit 1: Theories

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

Unit 2: Types of Reactions

Kinetics of chain reactions, detections of radical and kinetics of HBr, H₂O₂ 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 3: Electron Transfer Dynamics

Electron transfer in homogeneous systems, theory of electron transfer processes, electron tunneling, experimental results, electron transfer in heterogeneous systems, electrode- solution interface, rate of charge transfer in electrode reactions, study of kinetics of electrode processes.

Unit 4: 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. Radiation chemistry-Interaction with matter, dosimetry, and generation of free radicals and intermediated, comparison between photo- and radiation chemistry.

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.

8th Semester of Integrated M.Sc.

or

2nd Semester of 02 Year-M.Sc.

CYC-454: Structure and Properties of Metal Complexes

(Core Course: 03 Credits)

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 reactions 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 lasers.

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-carbonic anhydrase, carboxypeptidase, alcohol dehydrogenase, biological importance of Vitamin B12 and coenzyme.

Unit IV: 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

- [1] 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*”, 1 st Ed.. U.N. Dhur & Sons Pvt. Ltd., Calcutta, **1993**.
- [5] Lippard, S.J. and Berg, J., “*Principles of Bioinorganic Chemistry*”, University Science Books, U.S.A., **1994**.

8th Semester of Integrated M.Sc.

or

2nd Semester of 02 Year-M.Sc.

CYC-455: Instrumental Method of Analysis-II

(Core Course: 03 Credits)

Unit I: Vibrational Spectroscopy

Symmetry and shapes of AB₂, AB₃, AB₄, AB₅ and AB₆, 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 Fe²⁺, Fe³⁺, Sn²⁺ and Sn⁴⁺ compounds; detection of oxidation stated nature of M-L bond.

Unit IV: 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- finger print application, molecular weight determination.

Unit V:

Principles and Applications of XRD, XPS and PES.

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 N. Y. 1999.

8th Semester of Integrated M.Sc.

or

2nd Semester of 02 Year-M.Sc.

CYC-456: Inorganic Chemistry Lab-II

(Core Course: 02 Credits and 64 Contact Hours)

- [1] Comparison of electronic spectra of $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$, $[\text{Ni}(\text{NH}_3)_6]^{2+}$ and $[\text{Ni}(\text{en})_3]^{2+}$ and qualitative verification of the spectrochemical series, and quantitative estimation of nickel by spectrophotometry.
- [2] Synthesis and spectrophotometric study of copper complexes:
- Synthesis of bis(salicylaldehyde)copper(II) and cis-bis (glycinato)copper(II)
 - Record the spectra bis(salicylaldehyde)copper(II) and cis- bis (glycinato)copper(II), and
 - Record spectra of Cu^{2+} in water, NH_3 , ethylene diamine and glycine, and arrange the ligands in order of increasing field strength and
 - Quantitative estimation of copper by spectrophotometry or some other available technique.
- [3] (i) Study of the complex formation between Fe(III) and thiocyanate/salicylic acid/sulphosalicylic acid or between Ni(II) and o-phenanthroline, and
(ii) Spectrophotometric determination of formation of constant of the complex (Job's method and molar ratio method).
- [4] Synthesis of potassium tris(oxalate)aluminate, potassium tris(oxalate)chromate and potassium tris(oxalate)ferrate, and their characterization by metal determination, some spectroscopic methods, magnetic moment determination, and photochemical behaviour of iron complex.
- [5] Synthesis and characterization of $[\text{Co}(\text{en})_3]\text{Cl}_3$. Separation of its optical isomers and determination of their optical rotation by using a polarimeter.

Note: Minimum five experiments must be done and some experiments would require two-three turns.

Suggested Readings

- [1] Mendham, J., Denney, R.C., Barnes J.D. and Thomas M.J., "Vogel's Text Book of Quantitative Chemical Analysis", 6th Ed., ELBS Longman Group UK Ltd. (2004)
- [2] Vogel's *Qualitative Inorganic Analysis*, Revised by G. Svehla. Marr & Rockett "Inorganic Preparations"
- [3] Srivastava T.N. and Kamboj P.C., "Analytical Chemistry", Vishal Publications.
- [4] Marr & Rockett "Practical Inorganic Chemistry"

8th Semester of Integrated M.Sc.

or

2nd Semester of 02 Year-M.Sc.

CYC-457: Organic Chemistry Lab-II

(Core Course: 02 Credits and 60 Contact Hours)

- [1] Preparation of *p*-nitroaniline of acetanilide
- [2] Preparation of pyridium dichromate and its uses in oxidation of benzyl alcohol.
- [3] Cannizzaro reaction of an aromatic Aldehyde (*p*-nitrobenzaldehyde).
- [4] Synthesis of ω -nitrostyrene from an aromatic aldehyde and nitromethane
- [5] Synthesis of chalcone from an aromatic aldehyde and acetophenone.
- [6] Extraction of oils from ground nuts using soxhlet apparatus
- [7] Synthesis of α -bromo cinnamic acid or phenyl acetylene from benzaldehyde, (formation of cinnamic acid, bromination and elimination reactions).
- [8] Preparation of *meso*-stilbene dibromide and its conversion to diphenylacetylene.
- [9] Fisher indole synthesis.

Note: Minimum five experiments must be done and some experiments would require two-three turns.

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 (2012).

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2005

8th Semester of Integrated M.Sc.

or

2nd Semester of 02 Year-M.Sc.

CYC-458: Physical Chemistry Lab-II

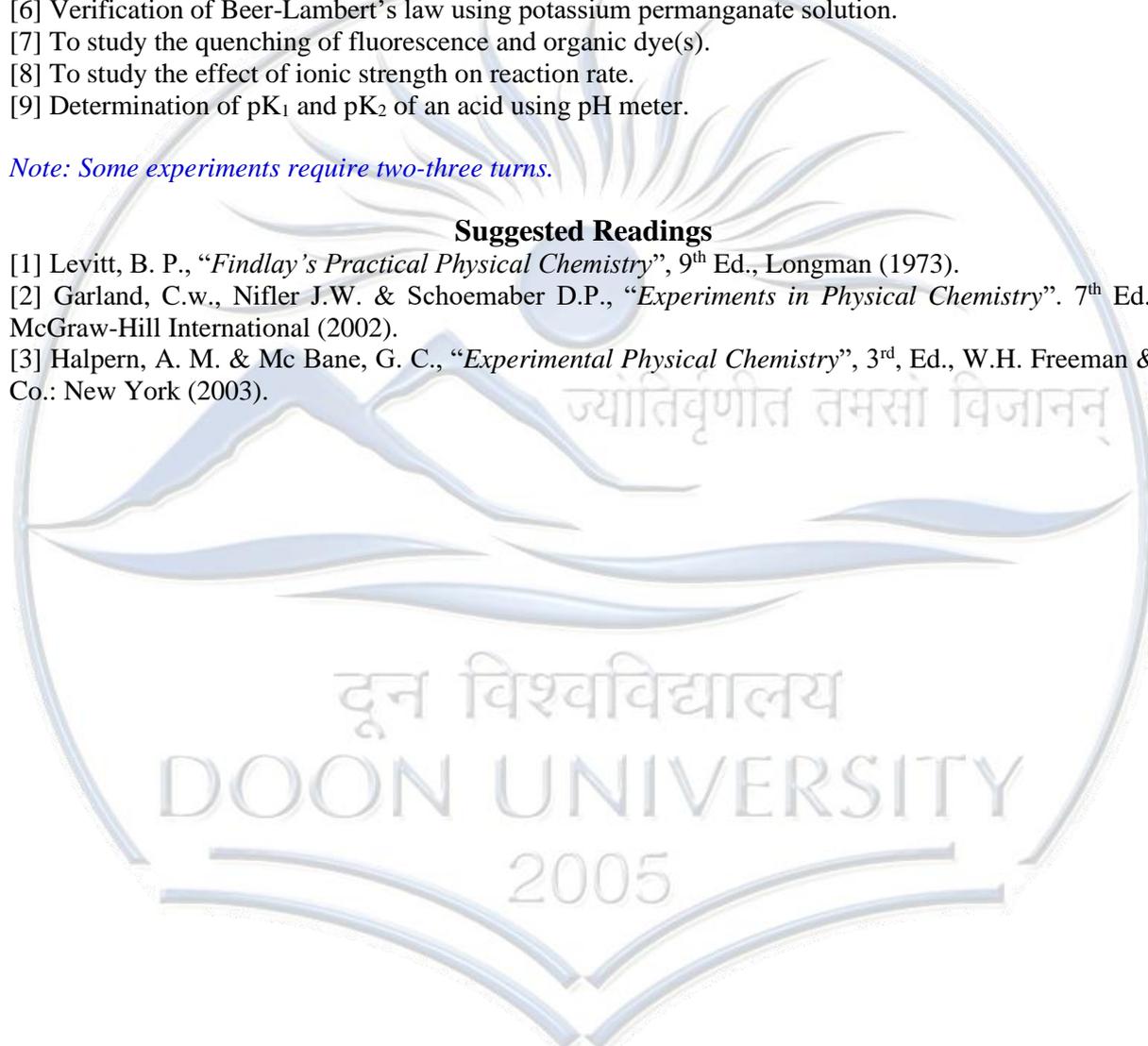
(Core Course: 02 Credits and 60 Contact Hours)

- [1] To study the kinetics of H⁺ catalyzed hydrolysis of an ester.
- [2] To study the kinetics of saponification of ester.
- [3] To study the kinetics of metal catalyzed decomposition of hydrogen peroxide.
- [4] To study the kinetics of inversion of sucrose using polarimeter
- [5] Determination of equilibrium constant of KI₃ complex by distribution method.
- [6] Verification of Beer-Lambert's law using potassium permanganate solution.
- [7] To study the quenching of fluorescence and organic dye(s).
- [8] To study the effect of ionic strength on reaction rate.
- [9] Determination of pK₁ and pK₂ of an acid using pH meter.

Note: Some experiments require two-three turns.

Suggested Readings

- [1] Levitt, B. P., "Findlay's Practical Physical Chemistry", 9th Ed., Longman (1973).
- [2] Garland, C.w., Nifler J.W. & Schoemaber D.P., "Experiments in Physical Chemistry". 7th Ed., McGraw-Hill International (2002).
- [3] Halpern, A. M. & Mc Bane, G. C., "Experimental Physical Chemistry", 3rd Ed., W.H. Freeman & Co.: New York (2003).



9th Semester of Integrated M.Sc.

or

3rd Semester of 02 Year-M.Sc.

Frontiers in Bioinorganic Chemistry

(Discipline Specific Elective Course: 03 Credits and 45 Contact Hours)

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 heme proteins with modified heme/other cofactors and their application in biocatalysis and electron transfer.

Unit III: Molybdenum and tungsten in biology:

Hyperthermophilic 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 synthase 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, manganese- 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, Inc., **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**.

9th Semester of Integrated M.Sc.

or

3rd Semester of 02 Year-M.Sc.

Frontiers in Bioinorganic Chemistry

(Discipline Specific Elective Course: 03 Credits and 45 Contact Hours)

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 radiative 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-excimer formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2'-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidizing character of Ru(II)-bipyridine 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 Inorganic 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] Coordination 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 Inorganic Photochemistry. G. J. Ferraudi, Wiley.

9th Semester of Integrated M.Sc.

or

3rd Semester of 02 Year-M.Sc.

Supramolecular Chemistry

(Discipline Specific Elective Course: 03 Credits and 45 Contact Hours)

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 acid-base concepts, enantio-selective anion recognition, 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.

9th Semester of Integrated M.Sc.

or

3rd Semester of 02 Year-M.Sc.

Advanced Quantum Chemistry

(Discipline Specific Elective Course: 03 Credits and 45 Contact Hours)

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 AH_n molecule: Methane, Ammonia and Water, Hybrid Orbitals: The Ethylene and Benzene Molecules.

Unit 6: Semiempirical Molecular Orbital Methods I - PI Electron Systems

The Hückel Approximation for Conjugated Hydrocarbons, The Pariser-Parr-Pople Method. Semiempirical Molecular Orbital Methods II - All valence – Electron systems: The Extended Hückel 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.

9th Semester of Integrated M.Sc.

or

3rd Semester of 02 Year-M.Sc.

Solid State Chemistry and Applications

(Discipline Specific Elective Course: 03 Credits and 45 Contact Hours)

Unit 1: 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, antiferite, nickel-arsenide, CaC₂, CdI₂ and TiO₂, FeTiO₃, MgAl₂O₄, Fe₂NiO₄, garnets, BaTiO₃ and KNiF₃. Non-ionic crystals– SiC, (BN)_x, giant molecules, layer structures, crystals composed of discrete molecules.

Unit 2: Defect structures

Thermodynamic defects and their consequences, solid electrolytes, non-stoichiometric compounds, F-centers and applications of defects in non-stoichiometric compounds.

Unit 3: 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 4: 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 5: 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 6: 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, solid 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.

9th Semester of Integrated M.Sc.

or

3rd Semester of 02 Year-M.Sc.

Advanced Surface and Colloidal Chemistry

(Discipline Specific Elective Course: 03 Credits and 45 Contact Hours)

Unit 1: 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 2: Membranes and their Applications

Artificial and natural membranes, Donnan membrane equilibrium, transport of electrolytes, membrane potential and ion selective electrodes.

Unit 3: 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 4: 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.

Unit 5: Macromolecules

Concepts of mass and number average molecular weights, methods of determining molecular weights (osmometry, viscometry, diffusion and light scattering method), sedimentation, fractional properties of macromolecules, statistical distribution of end-to-end dimension, calculation of average dimension of various chain structures.

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

9th Semester of Integrated M.Sc.

or

3rd Semester of 02 Year-M.Sc.

Environmental Pollutants and Analysis

(Discipline Specific Elective Course: 03 Credits and 45 Contact Hours)

Introduction:

Environmental Segments (Atmosphere, Hydrosphere, Lithosphere, Biosphere), Natural Cycles of the environment (The Hydrologic, Oxygen, Nitrogen, Phosphate and Sulphur Cycle), Commonly Used Terms

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

Analysis of trace pollutants in water (continued)

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 (ng l^{-1}) polychlorinated organic compounds

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, Chlorofluorocarbons and depletion of ozone layer, CFC substitutes, Consequences of ozone depletion, Photochemical smog, Chemical reactions involved in smog formation in the atmosphere, Organonitrogen compounds, Organic particles in the atmosphere, Nitrogen oxides in the atmosphere, Acid rain, Particles in the atmosphere.

Atmospheric Analysis-Gases:

Introduction, Determination of time-weighted average concentrations, Determination of inorganic gaseous pollutants, Determination of low-concentrations of organic pollutants, Desorption of the analyte, Determination of instantaneous concentrations, Chemiluminescence and fluorescence, Infrared spectrometry for carbon monoxide, Electrochemical sensors, 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 total organic content in the gas sample, Analysis of particulates after dissolution, Direct analysis of particulates, Drawbacks of the direct analysis.

Soil Formation

Introduction, Kinds of Rocks and Formation of Soil, Mineral components in soil

Soil properties:

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.

Toxicological Chemistry:

Toxic chemicals and toxicity, Kinetic phase and dynamic phase, Physiological responses to toxicants, Teratogenesis, mutagenesis and carcinogenesis, Toxicity of metals, inorganic compounds & organic compounds, Toxicity of some inorganic compounds

Toxicology of some organic compounds:

Benzene formaldehyde & acetaldehyde, polycyclic aromatic hydrocarbons (PAHs), phenols, Nitrosamines, Isocyanates and methyl isocyanates, Organophosphates and carbates, Inhibition by carbamate insecticide, Organochlorine compounds & PCBs, Dioxins and polychlorinated biphenyls, Polychlorinated biphenyls

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 HaJI of India (Private) Ltd., New Delhi, 1994.
- [7] J. Jeffrey Peirce., Ruth F. Weiner and P. Aame VesiliJld., 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] Vladimir 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.



9th Semester of Integrated M.Sc.

or

3rd Semester of 02 Year-M.Sc.

Macromolecules and Nanomaterials

(Discipline Specific Elective Course: Credits and Contact Hours)

Unit 1: 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 formation of microemulsion and their stability, Physical techniques, Applications.

Unit 2: 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. Interpenetrating networks (IPN), polymers, Polymers in biomedical applications - artificial organs and controlled drug delivery.

Unit 3: 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] Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing.
- [2] Heterogeneous Catalysis, C. Satterfield, 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- Francis)
- [9] Solid state and its applications by A.R. West.
- [10] New directions in solid state chemistry, J. Gopalakrishnan and C.N. R. Rao.
- [11] Principles of the solid state by HV Keer

Green Chemistry

(Discipline Specific Elective Course: 03 Credits and Contact Hours)

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.

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 benzoic 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, Cannizzaro reaction, Strecker synthesis, Reformatsky reaction.
- 4. Selective Methylation of Active Methylene Group using Dimethylcarbonate:** Solidstate polymerization of amorphous polymers using diphenylcarbonate; Use of "Clayon", a nonmetallic oxidative reagent for various reactions; Free Radical Bromination; Role of Tellurium in organic syntheses; Biocatalysis in organic syntheses.

Unit III: 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] V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, *Anamalaya Publishers* (2005).
- [2] P.T. Anastas & J.K. Warner: Oxford Green Chemistry- Theory and Practical, University Press (1998).
- [3] A.S. Matlack: Introduction to Green Chemistry, Marcel Dekker (2001).
- [5] M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).