FACULTY OF SCIENCES DEPARTMENT OF CHEMISTRY

**B.Sc. (Hons.) Chemistry** 

w.e.f. July 2019



## YMCA UNIVERSITY OF SCIENCE AND TECHNOLOGY



## YMCA UNIVERSITY OF SCIENCE AND TECHNOLOGY

## VISION

YMCA University of Science and Technology aspires to be a nationally and internationally acclaimed leader in technical and higher education in all spheres which transforms the life of students through integration of teaching, research and character building.

### **MISSION**

- To contribute to the development of science and technology by synthesizing teaching, research and creative activities.
- To provide an enviable research environment and state-of-the art technological exposure to its Scholars.
- To develop human potential to its fullest extent and make them emerge as world class leaders in their professions and enthuse them towards their social responsibilities



## HUMANITIES AND SCIENCES DEPARTMENT

## VISION

A department that can effectively harness its multidisciplinary strengths to create an academically stimulating atmosphere; evolving into a well-integrated system that synergizes the efforts of its competent faculty towards imparting intellectual confidence that aids comprehension and complements the spirit of inquiry.

## MISSION

- To create well-rounded individuals ready to comprehend scientific and technical challenges offered in the area of specialization.
- To counsel the students so that the roadmap becomes clearer to them and they have the zest to turn the blueprint of their careers into a material reality.
- To encourage critical thinking and develop their research acumen by aiding the nascent spirit for scientific exploration.
- Help them take economic, social, legal and political considerations when visualizing the role of technology in improving quality of life.
- To infuse intellectual audacity that makes them take bold initiatives to venture into alternative methods and modes to achieve technological breakthroughs.

#### **B.Sc. (Hons.) Chemistry**

Chemistry is one of the branches of science dealing with the structure and behavior of nature with molecular perspective to understand scientific reasoning. The course includes many concepts, such as Nano chemistry, supramolecular chemistry, quantum chemistry, biological chemistry etc. Chemistry is fast moving from being a descriptive field to an exact science, a transition that will increasingly require input from all branches of science.

Apart from chemistry, students will also be able to learn Physics, Mathematics and other subjects in this course. In addition, the well-equipped teaching and research laboratories will facilitate the students to develop experimental, analytical and conceptual skills and build their interest in the field of research.

The program and the curriculum are ideally designed for academic as well as research growth.

#### **PROGRAM OBJECTIVES**

- Producing graduates who are well grounded in the fundamentals of Chemistry and acquisition of the necessary skills, in order to use their knowledge in Chemistry in a wide range of practical application.
- Help to become creative chemist to become successful in a wide range of professions where logical approach is required.
- To create general understanding about different chemical interactions to build a solid foundation in the subject.
- Bachelor of Science in chemistry gives multiple career options for the students to their interest.
- To familiarize the student with different instruments like U.V. spectrophotometer, refractometer, pH meter polarometer

It also promotes research and creative activities of students by providing exposure to the realm of physical science and technical expertise. The B.Sc. (Hons.) programme in chemistry is designed to provide a thorough basic knowledge in Chemistry at the under graduate level. Apart from the general topics in Chemistry, many of the new topics included in the syllabus keeps the students abreast with the latest developments taking place in the field. Also the experiments chosen for each practical course is such that they bring out the concept of application of the theory in a practical situation. It also helps in creative thinking and self-learning.

#### **PROGRAM OUTCOMES**

After completion of the program, the students will:

- Have sufficient understanding of the basic concepts in chemical processes.
- Be able to learn computer Science/Mathematics/Chemistry/Electronics as an elective subject apart from Chemistry as a major subject.
- Be able to communicate effectively by oral, computing and graphical means.
- Become successful professionals by demonstrating logical and analytical thinking abilities.
- Enable to describe and apply the basic principles of chemistry and to carry out practical techniques important in chemical analysis.
- Provide a systematic understanding of core chemistry concepts, principles and theories along with their applications.

### YMCA UNIVERSITY OF SCIENCE AND TECHNOLOGY, FARIDABAD DEPARTMENT OF HUMANITIES AND SCIENCES

### STRUCTURE AND SYLLABI OF B.Sc. (Hons.) CHEMISTRY (6 SEMESTER COURSE)

Subject Code	Title	L	Т	Р	Internal Assessment	End- semester Examinati on	Total	Credits	Category Code
Discipline Co	ore Course (DCC) –	Comp	ulsory	7					
BCH 101	Inorganic Chemistry - I	4	0	0	25	75	100	4	DCC
BCH 102	Physical Chemistry - I	4	0	0	25	75	100	4	DCC
BCH 103	Inorganic Chemistry – I (Lab)	0	0	4	15	35	50	2	DCC
BCH 104	Physical Chemistry - I (Lab)	0	0	4	15	35	50	2	DCC
Ability Enha	ncement Compulsor	y Cour	se (A	ECC)	- Compulsory	·		·	
BENG 101	English	2	0	0	25	75	100	2	AEC
Open Electiv	ve Course (OEC-I) *	- Selec	et 1-pa	aper &	respective Lab(	if any) of the	followin	g 4-discipline	es
OMTH 101	Calculus/	5	1	0	25	75	100	6	OEC
OMTH 102	Basic Algebra	5	1	0	25	75	100	6	OEC
OCSC 101	Introduction to Programming	4	0	0	25	75	100	4	OEC
OPHY 101	Electricity & Magnetism	4	0	0	25	75	100	4	OEC
OCSC 102	Introduction to Programming (Lab)	0	0	4	15	35	50	2	OEC
OPHY 102	Electricity & Magnetism (Lab)	0	0	4	15	35	50	2	OEC
Massive Ope	en Elective Course (M	/00C	)**- (	Dnline	Compulsory Co	ourse in any o	ne semes	ter from Sem	-I to Sem-V
XXX	MOOC	4/6	0	0	25	75	100	4/6	MOOC
Total Credit	S							20	

#### SEMESTER I

## \* OEC- student has to choose one subject out of four disciplines and will be continue from Sem-I to Sem-IV.

\*\*The students have to pass at least one mandatory MOOC course with 4-6 credits (12-16 weeks) from the list given on the Swayam portal or the list given by the department/ university from 1<sup>st</sup> semester to  $3^{rd}$ semester as notified by the university. (Instructions to students overleaf) L - Lecture; T - Tutorial; P - Practical

## SEMESTER II

Subject Code	Title	L	Т	Р	Internal Assessmen t	End- semester Examinati on	Total	Credits	Category Code
Discipline C	ore Course (DCC) – C	ompi	ılsory	7					
BCH 201	Organic Chemistry - I	4	0	0	25	75	100	4	DCC
BCH 202	Physical Chemistry - II	4	0	0	25	75	100	4	DCC
BCH 203	Organic Chemistry – I Lab	0	0	4	15	35	50	2	DCC
BCH 204	Physical Chemistry – II Lab	0	0	4	15	35	50	2	DCC
Ability Enha	ncement Compulsory (	Cours	e (Al	ECC) – Co	ompulsory				
BEVS 101	Environmental Science	2	0	0	25	75	100	2	AEC
Open Electiv	ve Course (OEC-2) - Se	lect	l- pap	per & resp	ective Lab(if	any) of the f	ollowing d	lisciplines	•
OMTH 201	Linear Algebra	5	1	0	25	75	100	6	OEC
OMTH 202	Basic Calculus	5	1	0	25	75	100	6	OEC
OCSC 201	Introduction to Database System	4	0	0	25	75	100	4	OEC
OPHY 201	Mechanics	4	0	0	25	75	100	4	OEC
OCSC 202	Introduction to Database System (Lab)	0	0	4	15	35	50	2	OEC
OPHY 202	Mechanics (Lab)	0	0	4	15	35	50	2	OEC
Massive Ope	en Elective Course (MC	) ()	- Or	line Com	oulsory Cours	se in any one	e semester	from Sem-I to	Sem-V
XXX	MOOC	4/6	0	0	25	75	100	4/6	MOOC
Mandatory A	udit Course (MAC)								
XXX	Audit Course#	2	0	0	25	75	100	0	AUD
Total Credit	s							20	

# As per the list provided by University site

## SEMESTER III

		r –	1	1			T	1	
Subject Code	Title	L	Т	Р	Internal Assessment	End-semester Examination	Total	Credits	Category Code
Discipline Co	ore Course (DCC) – Com	puls	ory						
BCH 301	Inorganic Chemistry - II	4	0	0	25	75	100	4	DCC
BCH 302	Organic Chemistry - II	4	0	0	25	75	100	4	DCC
BCH 303	Physical Chemistry - III	4	0	0	25	75	100	4	DCC
BCH 304	Inorganic Chemistry – II Lab	0	0	4	15	35	50	2	DCC
BCH 305	Organic Chemistry – II Lab	0	0	4	15	35	50	2	DCC
BCH 306	Physical Chemistry – III Lab	0	0	4	15	35	50	2	DCC
Skill Enhance	ement Course (SEC) – Se	elect	1-pa	iper (	out of the follov	ving			
SECC 01	Basic Analytical Chemistry	2	0	0	25	75	100	2	SEC
SECC 02	Green Chemistry	2	0	0	25	75	100	2	SEC
SECC 03	Pharmaceutical chemistry	2	0	0	25	75	100	2	SEC
SECC 04	Pesticide Chemistry	2	0	0	25	75	100	2	SEC
SECC 05	Fuel Chemistry	2	0	0	25	75	100	2	SEC
Open Electiv	e Course (OEC-3) - Selec	ct 1-	pape	er &	respective Lab(	if any) of the follo	owing dis	sciplines	
OMTH 301	Differential Equations	5	1	0	25	75	100	6	OEC
OMTH 302	Statistics and Infinite Series	5	1	0	25	75	100	6	OEC
OCSC 301	Computer Networks & Internet Technology	4	0	0	25	75	100	4	OEC
OPHY 301	Waves & Optics	4	0	0	25	75	100	4	OEC
OCSC 302	Computer Networks &	0	0	4	15	35	50	2	OEC

Total Credit	s							26	
XXX	MOOC	4/ 6	0	0	25	75	100	4/6	MOOC
Massive Ope	n Elective Course (MOO	C) –	Onl	ine (	Compulsory Cou	irse in any one sen	nester fro	om Sem-I t	o Sem-V
OPHY 302	Waves & Optics (Lab)	0	0	4	15	35	50	2	OEC
	Internet Technology (Lab)								

#### Subject Title Р End-Total Credits L Т Internal Category Code semester Assessment Code Examinati on Discipline Core Course (DCC) - Compulsory BCH 401 Inorganic 4 0 0 25 75 100 4 DCC Chemistry - III BCH 402 4 0 0 25 75 100 4 DCC Organic Chemistry - III BCH 403 0 0 25 75 100 4 DCC 4 Physical Chemistry - IV BCH 404 0 0 4 15 35 50 2 DCC Inorganic Chemistry – III Lab **BCH 405** Organic 0 0 4 15 35 50 2 DCC Chemistry – III Lab **BCH 406** Physical 0 0 4 15 35 50 2 DCC Chemistry - IV Lab Skill Enhancement Course (SEC) - Select 1-paper out of the following (not opted in Sem-III) SECC 01 2 0 25 75 2 SEC 0 100 **Basic Analytical** Chemistry 2 25 75 2 SECC 02 0 0 100 SEC Green Chemistry SECC 03 Pharmaceutical 2 0 0 25 75 100 2 SEC chemistry 2 2 SECC 04 0 0 25 75 100 SEC Pesticide Chemistry 25 75 2 SECC 05 2 0 0 100 SEC Fuel Chemistry Open Elective Course (OEC-3) - Select 1- paper & respective Lab(if any) of the following disciplines **OMTH 401** Numerical 5 1 0 25 75 100 6 OEC Methods 5 0 25 75 6 **OMTH 402** Ordinary and 1 100 OEC Partial Differential Equations OCSC 401 Information 4 0 0 25 75 100 4 OEC Security 75 5 1 0 25 6 OEC **OPHY 401** Nuclear and 100 Particle Physics 0 2 **OCSC 402** Information 0 4 15 35 50 OEC Security (Lab)

#### SEMESTER IV

Massive (	Open Elective Cou	rse (MOOC	C) – (	Online	e Compulsor	ry Course in ar	y one semes	ter from Se	em-I to Sem-V
XXX	MOOC	4/6	0	0	25	75	100	4/6	MOOC
Total Cre	edits							26	

## SEMESTER V

Subject Code	Title	L	Т	Р	Internal Assessment	End- semester Examinati on	Total	Credits	Category Code
Discipline C	ore Course (DCC) -	- Comp	ulsory	7					
BCH 501	Organic Chemistry - IV	4	0	0	25	75	100	4	DCC
BCH 502	Physical Chemistry - V	4	0	0	25	75	100	4	DCC
BCH 503	Organic Chemistry – IV Lab	0	0	4	15	35	50	2	DCC
BCH 504	Physical Chemistry – V Lab	0	0	4	15	35	50	2	DCC
Discipline E	lective Course (DEC	C) selec	t any	2-pape	rs & respective	labs out of the	e followir	ng 3-papers	·
DECC 501	Analytical Chemistry	4	0	0	25	75	100	4	DEC
DECC 502	Polymer Chemistry	4	0	0	25	75	100	4	DEC
DECC 503	Cement Chemistry	4	0	0	25	75	100	4	DEC
DECC 504	Analytical Chemistry Lab	0	0	2	15	35	50	2	DEC
DECC 505	Polymer Chemistry Lab	0	0	2	15	35	50	2	DEC
DECC 506	Cement Chemistry Lab	0	0	2	15	35	50	2	DEC
Massive Ope	en Elective Course (	MOOC	C) – Oi	nline C	ompulsory Cou	rse in any one	e semeste	r from Sem-I	to Sem-V
XXX	MOOC	4/6	0	0	25	75	100	4/6	MOOC
Total Credit	ts							24	

## SEMESTER VI

Subject Code	Title	L	Т	Р	Internal Assessment	End- semester Examinati on	Total	Credits	Category Code
Discipline Co	ore Course (DCC) –	Compu	lsory	2-Pape	ers				
BCH 601	Inorganic Chemistry - IV	4	0	0	25	75	100	4	DCC
BCH 602	Organic Chemistry - V	4	0	0	25	75	100	4	DCC
BCH 603	Inorganic Chemistry – IV Lab	0	0	4	15	35	50	2	DCC
BCH 604	Organic Chemistry – V Lab	0	0	4	15	35	50	2	DCC
Discipline El	ective Course (DEC)	– Sele	ct an	y 2-pa	pers & respectiv	e lab (if any)	out of the	following 3-pa	apers
DECC 601	Medicinal Chemistry	4	0	0	25	75	100	4	DEC
DECC 602	Molecular Modeling & Drug Design	4	0	0	25	75	100	4	DEC
DECC 603	Research Methodology for Chemistry	5	1	0	25	75	100	6	DEC
DECC 604	Medicinal Chemistry Lab	0	0	2	15	35	50	2	DEC
DECC 605	Molecular Modeling & Drug Design Lab	0	0	2	15	35	50	2	DEC
Total Credit	s	•	•	•				24	

#### Grand Total Credits: 144/146 [140 + 4/6 (for MOOC Course)]

NOTE: 1. Discipline Elective Course (DEC) papers may be added or deleted as per UGC guidelines. 2. Skill Enhancement Course (SEC) papers may be added or deleted as per UGC guidelines.

#### Instructions to the students regarding MOOC

- 1. Two types of courses will be circulated: branch specific and general courses from the website <u>https://swayam.gov.in</u> in the month of June and November every year for the forthcoming semester.
- 2. The department coordinators will be the course coordinators of their respective departments.
- 3. Every student has to pass a selected MOOC course within the duration as specified below:

Programme	Duration
B. Tech.	Sem. I to Sem. VII
M.Sc./M.Tech./MA/MBA	Sem. I to Sem. III
B.Sc./MCA	Sem. I to Sem. V

The passing of a MOOC course is mandatory for the fulfilment of the award of the degree of concerned programme.

- 4. A student has to register for the course for which he is interested and eligible which is approved by the department with the help of course coordinator of the concerned department.
- 5. A student may register in the MOOC course of any programme. However, a UG student will register only in UG MOOC courses and a PG student will register in only PG MOOC courses.
- 6. The students must read all the instructions for the selected course on the website, get updated with all key dates of the concerned course and must inform his/her progress to their course coordinator.
- 7. The student has to pass the exam (online or pen-paper mode as the case may be) with at least 25% marks.
- 8. The students should note that there will be a weightage of Assessment/quiz etc. and final examination appropriately as mentioned in the instructions for a particular course.
- 9. A student must claim the credits earned in the MOOC course in his/her marksheet in the examination branch by forwarding his/her application through course coordinator and chairperson.

#### **Grading Scheme**

*Percentage	Grade	Grade Points	Category
≥90	0	10	Outstanding
$\geq$ 80 to < 90	<b>A</b> +	9	Excellent
$\geq$ 70 to < 80	Α	8	Very Good
$\geq$ 60 to < 70	<b>B</b> +	7	Good
$\geq$ 50 to < 60	В	6	Above average
$\geq$ 45 to < 50	С	5	Average
$\geq$ 40 to < 45	Р	4	Pass
< 40	F	0	Fail
	AB	0	Absent

#### \*Lower limit included, upper limit excluded

#### The multiplication factor for CGPA is 10

- 1. Automatic Rounding
- 2. Average difference between actual percentage and CGPA percentage  $\pm 2.5\%$
- 3. Worst case difference between actual percentage and CGPA percentage  $\pm$  5% if somebody in all the 8 semesters in all the exams (around 75 in numbers) consistently scores at the bottom of the range, say 55 of 55-65 which is a very remote possibility.

# SEMESTER I

#### Syllabus of B.Sc. (H) Chemistry

#### \_\_\_\_\_

Semester I

Paper: Inorganic Chemistry - I

Paper Code: BCH 101

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of atom and atomic structure, periodic properties of elements and chemical bonding.

Atomic Structure: Recapitulation of 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  $\psi$  and  $\psi^2$ . 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.

Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, aufbau principle and its limitations. (14 Lectures)

**Periodicity of Elements:** Brief discussion of the following properties of the elements, with reference to s & p-block and the trends shown:

- 1. Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.
- 2. Atomic and ionic radii.
- 3. Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization enthalpy and trends in groups and periods.
- 4. Electron gain entably and trends in groups and periods.
- 5. Electronegativity, Pauling's/ Allred Rochow's scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. (16 Lectures)

#### **Chemical Bonding:**

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.

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<sub>2</sub>, O<sub>2</sub>, C <sub>2</sub>, B<sub>2</sub>, F<sub>2</sub>, CO, NO, and their ions; HCl (idea of s-p mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of the following simple molecules and ions containing lone pairs and bond pairs of electrons: H<sub>2</sub>O, NH<sub>3</sub>, PCl<sub>3</sub>, PCl<sub>5</sub>, SF<sub>6</sub>, ClF<sub>3</sub>, I<sub>3</sub><sup>-</sup>, BrF<sub>2</sub><sup>+</sup>, PCl<sub>6</sub><sup>-</sup>, ICl<sub>2</sub><sup>-</sup>ICl<sub>4</sub><sup>-</sup> and SO<sub>4</sub><sup>2-</sup>, Multiple bonding 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.

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

Weak Chemical Forces: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interaction. Hydrogen bonding (theories of hydrogen bonding, valence bond treatment). Effects of weak chemical forces, melting and boiling points, solubility, energetics of dissolution process. (30 Lectures)

#### **Referred Books:**

- Lee, J.D. Concise Inorganic Chemistry, Pearson Education 2010
- Huheey, J.E., Keiter, E.A., Keiter, R. L., Medhi, O.K. Inorganic Chemistry, Principles of Structure and Reactivity, Pearson Education 2006.
- Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, Oxford, 1970
- Shriver, D.D. & P. Atkins, *Inorganic Chemistry* 2<sup>nd</sup> *Ed.*, Oxford University Press, 1994.
- Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications 1962.

Course Outcomes: After the completion of the course, students will be able to,

- Learn basic concept of atom and its structure in detail.
- Arrangement of electrons in atom.
- Concept of s, p, d and f orbitals and their shape using.
- Understand nature of chemical bonding and concept of molecular orbitals.

#### Paper: Inorganic Chemistry – I Lab Paper Code: BCH-103

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

#### (A) Titrimetric Analysis

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

#### **(B) Acid-Base Titrations**

Principles of acid-base titrations to be discussed.

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

#### (C) Oxidation-Reduction Titrimetry

Principles of oxidation-reduction titrations (electrode potentials) to be discussed.

- (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 K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> using internal indicator (diphenylamine, N-phenylanthranilic acid) and discussion of external indicator.

#### **Referred Books:**

• Vogel, A.I. A Textbook of Quantitative Inorganic Analysis, ELBS.

#### Paper: Physical Chemistry - I

Paper Code: BCH-102

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the different states of matter and various laws governing the properties of solid, liquid and gaseous state. Emphasis will also be on the basic concept of ionic equilibrium and its applications.

**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  $\zeta$  from  $\eta$ ; 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 and temperature for different gases. Causes of deviation from ideal behaviour. van der Waals equation of state, its derivation and application in explaining real gas behaviour, 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. (18 Lectures)

**Liquid state:** Qualitative treatment of the structure of the liquid state; 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. (6 Lectures)

**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.

(16 Lectures)

**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 and diprotic acids. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications. 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. **(20 Lectures)** 

Course Outcomes: After the completion of the course, students will be able to,

- Learn the states of matter in detail.
- Laws governing the solid, liquid and gaseous state.
- Have a deep understanding methods to study the solid, liquid and gaseous state.
- Concept of ionic equilibria and its applications.

#### **Reference Books:**

- Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry Ed., Oxford University Press 13 (2006).
- Ball, D. W. Physical Chemistry Thomson Press, India (2007).
- Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).
- Mortimer, R. G. Physical Chemistry 3rd Ed. Elsevier: NOIDA, UP (2009).

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## Paper: Physical Chemistry – I (Lab) Paper Code: BCH-104

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

#### 1. Surface tension measurements using stalagmometer.

a. Determine the surface tension by (i) drop number (ii) drop weight method.

b. Study the variation of surface tension with different concentration of detergent solutions. Determine CMC.

#### 2. Viscosity measurement using Ostwald's viscometer.

a. Determination of co-efficient of viscosity of an unknown aqueous solution.

b. Study the variation of co-efficient of viscosity with different concentration of Poly Vinyl Alcohol (PVA) and determine molar of PVA.

c. Study the variation of viscosity with different concentration of sugar solutions.

#### 3. Solid State:

a. Indexing of a given powder diffraction pattern of a cubic crystalline system.

#### 4. pH metry:

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

Any other experiment carried out in the class.

#### **Reference Books**

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

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

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

## **SEMESTER II**

Semester II

Paper: Organic Chemistry - I Paper Code: BCH-201

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to have an understanding the structure and bonding in organic chemistry, electronic displacements, stereochemistry and chemistry of aliphatic and aromatic hydrocarbons.

#### **Recapitulation of basics of Organic Chemistry**

Hybridization, Shapes of molecules

Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation Dipole moment; Hydrogen bonding (Applications to be discussed with relevant topics)

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

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

(6 Lectures)

#### **Stereochemistry:**

Fischer,Newmann and Sawhorse Projection formulae and their interconversions; Geometrical isomerism: cis–trans, syn-anti and 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 their resolution. Relative and absolute configuration: D/L and R/S designations.

(18 Lectures)

#### **Chemistry of Aliphatic Hydrocarbons**

#### A. Carbon-Carbon sigma bonds

General methods of prepareation, physical and chemical properties of alkanes: Wurtz Reaction, Wurtz-Fittig Reactions, Free radical substitutions: Halogenation -relative reactivity and selectivity.

#### **B.** Carbon-Carbon pi bonds:

General methods of preparation, physical and chemical properties of alkenes and alkynes, Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations. Electrophilic additions their mechanisms (Markownikoff/ Anti Markownikoff addition), mechanism of oxymercuration-demercuration, hydroboration- oxidation, 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

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

(24 Lectures)

#### 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. (12 Lectures)

Course Outcomes: After the completion of the course, students will be able to,

- Know the basic concepts of organic chemistry.
- Understand the basics of reaction mechanism.
- Stereochemistry and optical isomerism in organic compounds.
- Understand the chemistry of aliphatic and aromatic hydrocarbons.

#### **Reference Books:**

- Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds; Wiley: London, 1994.
- Kalsi, P. S. Stereochemistry Conformation and Mechanism; New Age International, 2005.

#### Paper: Organic Chemistry – I (Lab)

#### Paper Code: BCH-203

No. of Credits: 4 L: 4, T: 0 60 Periods Internal: 15 External Exam: 35 Total: 50

- 1. Checking the calibration of the thermometer
- Purification of organic compounds by crystallization using the following solvents:

   a.Water
   b.Alcohol
   c.Alcohol-Water
- 3. Determination of the melting points of 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)

- 7. Detection of extra elements
- 8. Organic Preparations
  - (i) Bromination of acetanilide / aniline / phenol
  - (ii) Nitration of nitrobenzene / toluene.

#### **Reference Books:**

- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)

Paper: Physical Chemistry - II

Paper Code: BCH-202

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to have an understanding concept of thermodynamics in chemistry, system of variable composition, chemical equilibrium, solutions and colligative properties.

**Chemical Thermodynamics:** Intensive and extensive variables; state and path functions; isolated, closed and open systems.

**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,  $\Delta U$  and  $\Delta H$  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 and enthalpy of combustion and its applications; effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions.

**Second Law:** Concept of entropy; thermodynamic scale of temperature, statement of the second law of thermodynamics. 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. (36 Lectures)

**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. (8 Lectures)

**Chemical Equilibrium:** Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration ( Le Chatelier Principle, Quantitatively)). Free energy of mixing and spontaneity. equilibrium between ideal gases and a pure condensed phase. (8 Lectures)

**Solutions and Colligative Properties:** Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Thermodynamic derivation using chemical potential to

derive relations between the four colligative properties [(i) relative lowering of vapour pressure, 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. (8 Lectures)

Course Outcomes: After the completion of the course, students will be able to,

- Understand the basic concept of chemical thermodynamics and the laws governing.
- Learn the basics of systems of variable compositions.
- Learn the concept of chemical equilibrium.
- Learn solution and colligative properties.

#### **Reference Books**

• Peter, A. & Paula, J. de. Physical Chemistry 9th Ed., Oxford University Press (2011).

- Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
- Rastogi, R.P and Mishra, R.R. An introduction to chemical Thermodynamics, 1995.

• Kapoor, K.L., A text book of physical chemistry, vol 2, McGraw Hill education

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• Levine, I .N. Physical Chemistry 6th Ed., Tata Mc Graw Hill (2010). • Metz, C.R. 2000 solved problems in chemistry, Schaum Series (2006)

#### Paper: Physical Chemistry - II (Lab)

#### Paper Code: BCH-204

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

(a) Determination of heat capacity of a calorimeter for different volumes using (i) change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution of sulphuric acid or enthalpy of neutralization), and (ii) heat gained equal to heat lost by cold water and hot water respectively

(b) etermination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.

(c) Determination of the enthalpy of ionization of ethanoic acid.

(d) Determination of integral enthalpy (endothermic and exothermic) solution of salts.

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

(f) Determination of enthalpy of hydration of salt.

(g) Study of the solubility of benzoic acid in water and determination of  $\Delta H$ .

Any other experiment carried out in the class.

#### **Reference Books**

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

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# SEMESTER III

#### Syllabus of B.Sc. (H) Chemistry

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Semester III

Paper: Inorganic Chemistry - II

Paper Code: BCH 301

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of s & p block elements and the concept of metallurgy.

#### **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 with reference to cyanide process for silver and gold. Methods of purification of metals: Electrolytic process, van Arkel-de Boer process and Mond's process, Zone refining. (6 Lectures)

#### Chemistry of *s* Block Elements:

- (i) General characteristics: melting point, flame colour, reducing nature, diagonal relationships and anomalous behavior of first member of each group.
- (ii) Reactions of alkali and alkaline earth metals with oxygen, hydrogen, nitrogen and water.
- (iii) Common features such as ease of formation, thermal stability and solubility of the following alkali and alkaline earth metal compounds: hydrides, oxides, peroxides, superoxides, carbonates, nitrates, sulphates.
- (iv) Complex formation tendency of s-block elements; structure of the following complexes: crown ethers and cryptates of Group I; basic beryllium acetate, beryllium nitrate, EDTA complexes of calcium and magnesium.
- (v) Solutions of alkali metals in liquid ammonia and their properties. (22 Lectures)

#### Chemistry of *p* Block Elements:

Electronic configuration, atomic and ionic size, metallic/non-metallic character, melting point, ionization enthalpy, electron gain enthalpy, electronegativity, Allotropy of C, P, S; inert pair effect, diagonal relationship between B and Si and anomalous behaviour of first member of each group. (6 lectures)

Structure, bonding and properties: acidic/basic nature, stability, ionic/covalent nature, oxidation/reduction, hydrolysis, action of heat of the following:

- •Hydrides: hydrides of Group 13 (only diborane), Group 14, Group 15 (EH<sub>3</sub> where E = N, P, As, Sb, Bi), Group 16 and Group 17.
- •Oxides: oxides of phosphorus, sulphur and chlorine
- •Oxoacids: oxoacids of phosphorus and chlorine; peroxoacids of sulphur
- •Halides: halides of silicon and phosphorus

Preparation, properties, structure and uses of the following compounds:

- •Borazine
- •Silicates, silicones,
- Phosphonitrilic halides  $\{(PNCl_2)_n \text{ where } n = 3 \text{ and } 4\}$
- Interhalogen and pseudohalogen compounds
- •Clathrate compounds of noble gases, xenon fluorides (MO treatment of XeF<sub>2</sub>).

(26 Lectures)

#### **Referred Books:**

- Lee, J.D. Concise Inorganic Chemistry, Pearson Education 2010
- Lee, J.D. Concise Inorganic Chemistry, Pearson Education 2010
- Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. Concepts & Models of Inorganic Chemistry 3<sup>rd</sup> Ed., John Wiley Sons, N.Y. 1994.
- Cotton, F.A. & Wilkinson, G. Advanced Inorganic Chemistry, Wiley, VCH, 1999.
- Greenwood, N.N. & Earnshaw. Chemistry of the Elements, Butterworth-Heinemann. 1997.
- Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry* 3<sup>rd</sup> Ed.(adapted), Pearson, 2009
- Shriver, D.F., Atkins P.W and Langford, C.H., *Inorganic Chemistry* 2<sup>nd</sup> Ed., Oxford University Press, 1994

Course Outcomes: After the completion of the course, students will be able to,

- Understand general principles of metallurgy.
- Understand general characteristics and chemical properties of s & p block elements.
- Learn chemical and physical properties of hydrides, oxides, oxo and halides of various groups.
- Understand preparation, properties, structures of borazines, silicates, silicons, phosphonitrilic halides, interhalogens and pseudohalogen compounds and clatherate compounds of nobel gases.

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#### Paper: Inorganic Chemistry – II Lab Paper Code: BCH-304

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

#### (A) Iodo/Iodimetric Titrations

- (i) Estimation of Cu(II) and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> using sodium thiosulphate solution (Iodometrically).
- (ii) Estimation of antimony in tartar-emetic iodimetrically

#### (B) Complexometric titrations using disodium salt of EDTA

- (i) Estimation of  $Mg^{2+}$ ,  $Zn^{2+}$
- (ii) Estimation of Ca<sup>2+</sup>

#### (C) Inorganic preparations

- (i) Cuprous Chloride, Cu<sub>2</sub>Cl<sub>2</sub>
- (ii) Manganese(III) phosphate, MnPO<sub>4</sub>.H<sub>2</sub>O
- (iii)Aluminium potassium sulphate KAl(SO<sub>4</sub>)<sub>2</sub>.12H<sub>2</sub>O (Potash alum) or Chrome alum.

#### **Referred Books:**

- Vogel, A.I. A Textbook of Quantitative Inorganic Analysis, ELBS.
- Marr, G. and Rockett, R.W. *Practical Inorganic Chemistry*, Van Nostrand Reinhold. 1972.

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#### Paper: Organic Chemistry - II

Paper Code: BCH 302

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of some of the functional group chemistry, their methods of synthesis and chemical reactions.

#### **Chemistry of Halogenated Hydrocarbons:**

Alkyl halides: Methods of preparation and properties, nucleophilic substitution reactions - S<sub>N</sub>1,

S<sub>N</sub>2 and S<sub>N</sub>i mechanisms with stereochemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination.

Aryl halides: Preparation ( including preparation from diazonium salts) and properties, nucleophilic aromatic substitution; SNAr, Benzyne mechanism.

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

Organometallic compounds of Mg (Grignard reagent) – Use in synthesis of organic compounds. (16 Lectures)

#### Alcohols, Phenols, Ethers and Epoxides:

*Alcohols:* preparation, properties and relative reactivity of  $1^{\circ}$ ,  $2^{\circ}$ ,  $3^{\circ}$  alcohols, Bouvaelt-BlancReduction; Oxidation of diols 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<sub>4</sub> (16 Lectures)

#### **Carbonyl Compounds:**

Structure, reactivity, preparation and properties; Nucleophilic additions, Nucleophilic additionelimination reactions with ammonia derivatives with mechanism; Keto-enol tautomerism and concept of enol chemistry, Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisan-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann rearrangement, haloform reaction, Baeyer Villiger oxidation, Clemmensen, Wolff-Kishner and Meerveing Pondorf Verley reduction.

Addition reactions of  $\alpha$ ,  $\beta$ - unsaturated carbonyl compounds: Michael addition.

Active methylene compounds: Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate. (16 Lectures)

# **Carboxylic Acids and their Derivatives:**

General methods of preparation, physical properties and reactions of monocarboxylic acids, effect of substituents on acidic strength. Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids.

Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilicsustitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann- bromamide degradation and Curtius rearrangement. (12 Lectures)

# **Referred Books:**

- Morrison, R.T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd.
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
- Norman, R.O.C. & Coxon, J. M. Principles of Organic synthesis.

Course Outcomes: After the completion of the course, students will be able to,

- Perform inter-conversions of various functional groups in organic chemistry.
- Learn the carbon-carbon bond formations, redox reactions with mechanistic understanding.
- Understand the stereochemical aspect of reaction mechanism.
- Learn the properties, synthesis and chemical reactions of halogen and/or oxygen containing functional groups in organic chemistry.

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# Paper: Organic Chemistry – II Lab Paper Code: BCH-305

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

# A. Functional group tests for alcohols, phenols, carbonyl and carboxylic acid group.

# **B.** Organic preparations:

- i. Acylation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p- anisidine) and one of the following phenols ( $\beta$  -naphthol, resorcinol, p- cresol).
- ii. Oxidation of ethanol/ isopropanol (Iodoform reaction).
- iii. Selective reduction of meta dinitrobenzene to m-nitroaniline.
- iv. Hydrolysis of amides and esters.
- v. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.
- vi. S-Benzylisothiouronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
- vii. Aldol condensation using either conventional or green method.

(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 and melting point.)

# **Referred Books:**

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

38

#### Paper: Physical Chemistry - III

Paper Code: BCH 303

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of phase equilibria, electrochemical cells and surface chemistry.

**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 (H<sub>2</sub>O and S), with applications. Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points. Three component systems: triangular plots, water-chloroform-acetic acid system. Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and non ideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation. Nernst distribution law: its derivation and applications.

#### (27 Lectures)

### **Electrochemical Cells and Batteries:**

Rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry. Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and SbO/Sb<sub>2</sub>O<sub>3</sub> 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), Primary and secondary batteries.

#### (27 Lectures)

**Surface chemistry:** Physical adsorption, chemisorption, adsorption isotherms (Langmuir and Freundlich). nature of adsorbed state. (6 Lectures)

# **Referred Books:**

- Peter Atkins & Julio De Paula, Physical Chemistry 9th Ed., Oxford University Press (2010).
- Castellan, G. W. Physical Chemistry, 4th Ed., Narosa (2004).
- Puri,B.R., Sharma,L.R., Pathania,M.S., Principles of Physical chemistry,Vishal Publicating Co., 2016
- Zundhal, S.S. Chemistry concepts and applications Cengage India (2011).
   Ball, D. W. Physical Chemistry Cengage India (2012).
- Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009). Levine, I. N. Physical Chemistry 6th Ed., Tata McGraw-Hill (2011).
- Metz, C. R. Physical Chemistry 2nd Ed., Tata McGraw-Hill (2009).

Course Outcomes: After the completion of the course, students will be able to,

- Learn basic concept of phase equilibria and their applications.
- Understand the qualitative and quantitative aspects of electrochemical cells.
- Understand the nature of adsorption and their qualitative analysis.
- Learn analytical concepts of various reactions through potentiometric titrations.

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# Paper: Physical Chemistry – III Lab Paper Code: BCH-306

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

# Phase Equibria:

- I. Determination of critical solution temperature and composition at CST of the phenolwater system and to study the effect of impurities of sodium chloride and succinic acid 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 chloroform or cyclohexane.
- IV. Study the equilibrium of at least one of the following reactions by the distribution method:
  - (i)  $I_2(aq) + I^-(aq) \rightarrow I_3^-(aq)$
  - (ii)  $\operatorname{Cu}^{2+}(\operatorname{aq}) + \operatorname{nNH}_3 \rightarrow \operatorname{Cu}(\operatorname{NH}_3) \operatorname{n}^{2+}$

# **Potentiometry:**

V. 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

#### **Adsoption:**

I. Verify the Freundlich and Langmuir isotherms of acetic acid on activated charcoal.

# **Referred Books:**

- Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011). 25
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.;
   W.H. Freeman & Co.: New York (2003).

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#### Syllabus of B.Sc. (H) Chemistry

#### Semester III & IV– Skill Enhancement Course

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Basic Analytical Chemistry Paper Code: SECC 01

No. of Credits: 2 L: 2, T: 0 Theory: 30 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of sampling and analysis of soil, water, gasoline, arson accelerants by different analytical techniques, spectrophotometric study of tablets and soft drinks.

**Introduction:** Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. Presentation of experimental data and results, from the point of view of significant figures.

**Analysis of soil**: Composition of soil, Concept of pH and pH measurement, Complexometric titrations, Chelation, Chelating agents, use of indicators

- (i) Determination of pH of soil samples.
- (ii) Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

**Analysis of water:** Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.

- (i) Determination of pH, acidity and alkalinity of a water sample.
- (ii) Determination of dissolved oxygen (DO) of a water sample. (15 Lectures)

**Chromatography:** Definition, general introduction on principles of chromatography, paper chromatography, TLC etc. Separation of a mixture of different metal ions (Ni<sup>2+</sup> and Co<sup>2+</sup>) by paper chromatography.

**Ion-exchange:** Column, ion-exchange chromatography etc. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Suggested Applications (Any one):

- a. To study the use of phenolphthalein in trap cases.
- b. To analyze arson accelerants.
- c. To carry out analysis of gasoline.

Suggested Instrumental demonstrations:

- a. Estimation of macro nutrients: Potassium, Calcium, Magnesium in soil samples by flame photometry.
- b. Spectrophotometric determination of Iron in Vitamin / Dietary Tablets.
- c. Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in Soft Drink. (15 Lectures)

(Demonstration will be given through audio visual aids.)

# **Referred Books:**

- Willard, H. H. Instrumental Methods of Analysis, CBS Publishers, 1988.
- Skoog, D.A. and Leary, J.J., *Instrumental Methods of Analysis*, Saunders College Publications, New York, 1992
- Skoog, D.A.; West, D.M. and Holler, F.J. *Fundamentals of Analytical Chemistry* 6<sup>th</sup> Ed., Saunders College Publishing, Fort Worth, 1992
- Harris, D. C. *Quantitative Chemical Analysis* 7<sup>th</sup> Ed., W. H. Freeman and Co., New York, 2007
- Dean, J. A. Analytical Chemistry Handbook, McGraw Hill, 2007
- Day, R. A. and Underwood, A. L. *Quantitative Analysis*, Prentice Hall of India, 1991Freifelder, D. *Physical Biochemistry* 2<sup>nd</sup> Ed., W.H. Freeman and Co., N.Y. 1982
- Cooper, T.G. (Ed.) The Tools of Biochemistry, John Wiley and Sons, N.Y. 1977
- S v e h l a , G . , Vogel's Qualitative Inorganic Analysis 7<sup>th</sup> Ed., Prentice Hall, 1996
- Mendham, J., Denney, R.C., Barnes, J.D. and Thomas, M.J.K., Vogel's Quantitative
- *Chemical Analysis 6<sup>th</sup> Ed.*, Prentice Hall, 2007.
- Robinson, J.W. Undergraduate Instrumental Analysis 5<sup>th</sup> Ed., Marcel Dekker, Inc., New York, 1995.

- Understand sampling presentation of experimental data and results.
- Analyse soil and water samples.
- Learn different chromatographic techniques.
- Handel different analytical instruments.

Green Chemistry Paper Code: SECC 02

No. of Credits: 2 L: 2, T: 0 Theory: 30 Lectures Sessional: 25 Theory Exam: 75 Total: 100

### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of Green Chemistry and its applications to sustainable development.

# **Theory and Hands-on Experiments**

Introduction: Definitions of Green Chemistry. Brief introduction of twelve principles of Green Chemistry, with examples, special emphasis on atom economy, reducing toxicity, green solvents, Green Chemistry and catalysis and alternative sources of energy, Green energy and sustainability

### The following Real world Cases in Green Chemistry should be discussed:

- 1 Surfactants for Carbon Dioxide replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments.
- 2 Designing of Environmentally safe marine antifoulant.
- 3 Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
- 4 An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn. (20 Lectures)

# **Practicals:**

- 1 Preparation and characterization of biodiesel from vegetable oil.
- 2 Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared from dry ice.
- 3 Mechanochemical solvent free synthesis of azomethine.
- 4 Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper(II) (20 Lectures)

# **Referred Books:**

- Anastas, P.T. and Warner, J.K. Oxford Green Chemistry- Theory and Practical, University Press, 1998
- Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker, 2001
- Cann, M.C. and Connely, M.E., *Real-World Cases in Green Chemistry*, American Chemical Society, Washington, 2000
- Ryan, M.A. and Tinnesand, M., *Introduction to Green Chemistry*, American Chemical Society, Washington, 2002.

- Sharma, R.K., Sidhwani, I.T. and Chaudhari, M.K. *Green Chemistry Experiments: A monograph*, I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore ISBN 978-93-81141-55-7, 2013
- Lancaster, Mike Green Chemistry: An Introductory Text 2<sup>nd</sup> Ed., RSC Publishing, ISBN 978-1-84755-873-2, 2010
- Wealth from waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated A social Awareness Project
- Indu Tucker Sidhwani, Geeta Saini, Sushmita Chowdhury, Dimple Garg, Malovika, Nidhi Garg, Delhi University Journal of Undergraduate Research and Innovation, Vol1, Issue 1, Feb 2015. ISSN: 2395-2334.

Course Outcomes: After the completion of the course, students will be able to,

- Understand the concept of Green Chemistry.
- To perform green synthesis of surfactants, rightfit pigments and compostable plastic like polylactic acid.
- Understand the practical aspect of preparation of biodiesel, extraction of D-limonene etc. Concept of s, p, d and f orbitals and their shape using.
- Understand the importance of Green Chemistry for sustainable development.

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# Pharmaceutical Chemistry Paper Code: SECC 03

No. of Credits: 2 L: 2, T: 0 Theory: 30 Lectures Sessional: 25 Theory Exam: 75 Total: 100

### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of drug designing and their synthesis.

# **Drugs & Pharmaceuticals**

An elementary idea of medicinal values of curcumin (Haldi), Azadirachtin (Neem), Withania Somnifera (Aswagandha), ocimum sanclum (Tulsi), Aloe Vera. Drug discovery, design and development; Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (paracetamol, lbuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphanethoxazol, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT-Zidovudine). (15 Lectures)

#### 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).

(15 Lectures)

(Demonstration of basic idea of drug action and their interaction with receptors through audio visual aids)

# **Referred Books:**

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

Course Outcomes: After the completion of the course, students will be able to,

• Learn drug design and development.

- Understand drugs functionality.
- Understand the methods of synthesis of various drugs.
- Learn the concept of fermentation.

# Pesticide Chemistry Paper Code: SECC 04

No. of Credits: 2 L: 2, T: 0 Theory: 30 Lectures Sessional: 25 Theory Exam: 75 Total: 100

# **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of manufacturing and use of pesticides.

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

Harmful effects of overuse of pesticides and the concept of biomagnifications.

The concept of integrated pest management and its significance over using chemical based pest. (20 Lectures)

# **Practicals**

- (i) To calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
- (ii) Preparation of simple organophosphates, phosphonates and thiophosphates

# (15Lectures)

# **Referred Books:**

• R. Cremlyn: Pesticides, John Wiley.

Course Outcomes: After the completion of the course, students will be able to,

- Understand the chemistry of pesticides.
- Learn benefits and adverse effects of pesticides.
- Understand biomagnifications and integrated pest management.

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# Fuel Chemistry Paper Code: SECC 05

No. of Credits: 2 L: 2, T: 0 Theory: 30 Lectures Sessional: 25 Theory Exam: 75 Total: 100

### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the classification of fuels and lubricants and their chemical and physical properties.

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

Coal: Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal.Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar bases chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Petroleum and Petrochemical Industry: Composition of crude petroleum, Refining and different types of petroleum products and their applications. (15 Lectures)

Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), 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. Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene.

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) and their determination (15 Lectures)

# **Referred Books:**

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

- Classify fuels alongwith their calorific values.
- Understand coal chemistry
- Learn recovery of petroleum products by various processes.
- Learn lubricant classifications and its applications.

# SEMESTER IV

#### Syllabus of B.Sc. (H) Chemistry

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Semester IV

Paper: Inorganic Chemistry - III

Paper Code: BCH 401

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the coordination chemistry, study of dblock elements, actinoides and lanthanoides.

### **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 ( $\Delta$ o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq ( $\Delta$ o,  $\Delta$ 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. (26 Lectures)

#### **Substitution reactions**

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar and octahedral complexes, Trans- effect, theories of trans effect. (10 Lectures)

# **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 diagrams) Different between the first, second and third transition series.

Chemistry of Cr, Mn, Fe and Co in various oxidation states with special reference to the following compounds: peroxo compounds of chromium, potassium dichromate, potassium

permanganate, potassium ferrocyanide, potassium ferricyanide, sodium nitroprusside and sodium cobaltinitrite. (16 Lectures)

# Lanthanoids and Actinoids:

Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only). (8 Lectures)

# **Referred Books:**

- Purcell, K.F & Kotz, J.C., Inorganic Chemistry W.B. Saunders Co, 1977.
- Huheey, J.E., Inorganic Chemistry, Prentice Hall, 1993.
- Cotton, F.A. & Wilkinson, G., Advanced Inorganic Chemistry Wiley-VCH, 1999
- Basolo, F, and Pearson, R.C., *Mechanisms of Inorganic Chemistry*, John Wiley & Sons, NY, 1967.
- Greenwood, N.N. & Earnshaw A., *Chemistry of the Elements*, Butterworth-Heinemann, 1997.
- Miessler, G. L. &. Tarr, Donald A. Inorganic Chemistry 3<sup>rd</sup> Ed.(adapted), Pearson, 2009

- Learn coordination chemistry of transition metal complexes.
- Understand the chemistry of d-block elements.
- Understand chemistry of lanthanoides and actinoides.
- Learn the basics of inorganic reaction mechanism.

# Paper: Inorganic Chemistry – III Lab Paper Code: BCH-404

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

# **Gravimetric Analysis:**

- i. Estimation of nickel (II) using Dimethylglyoxime (DMG).
- ii. Estimation of copper as CuSCN
- iii. Estimation of iron as Fe<sub>2</sub>O<sub>3</sub> by precipitating iron as Fe<sub>(OH)3</sub>.
- iv. Estimation of Al(III) by precipitating with oxine and weighing as Al(oxine)<sub>3</sub> (aluminium oxinate).

# **Inorganic Preparations:**

- i. Tetraamminecopper (II) sulphate, [Cu(NH3)4]SO4.H2O
- ii. Acetylacetonate complexes of  $Cu^{2+}/Fe^{3+}$
- iii. Tetraamminecarbonatocobalt (III) nitrate
- iv. Potassium tri(oxalato)ferrate(III)

# **Properties of Complexes**

- i. Measurement of 10 Dq by spectrophotometric method
- ii. Verification of spectrochemical series.

# Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method

# **Referred Books:**

- Vogel, A.I. A Textbook of Quantitative Inorganic Analysis, ELBS.
- G. Marr and B.W. Rockett, Practical Inorganic Chemistry, Van Nostrand Reinhold. 1972

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Paper: Organic Chemistry - III Paper Code: BCH 402

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the properties, synthesis and chemical reactions of nitrogen containing functional groups, polynuclear hydrocarbons, heterocyclic compounds and alkaloids.

### **Nitrogen Containing Functional Groups**

Preparation and important reactions of nitro compounds, nitriles and isonitriles. Amines: Preparation and properties: Effect of substituent and solvent on basicity; 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. (18 Lectures)

#### **Polynuclear Hydrocarbons**

Aromaticity of polynuclear hydrocarbons, structure elucidation of naphthalene; Preparation and properties of naphthalene, phenanthrene and anthracene. (6 Lectures)

#### **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), Indole(Fischer indole synthesis and Madelung synthesis), Quinoline and isoquinoline, (Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner- Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch reaction). (22 Lectures)

#### Alkaloids

Natural occurrence, General structural features, Isolation and their physiological action,Hoffmann's exhaustive methylation, Emde's modification; Structure elucidation and synthesis of Nicotine. Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine, and Reserpine. (7 Lectures)

#### Terpenes

Occurrence, classification, isoprene rule; Elucidation of stucture and synthesis of Citral.

(7 Lectures)

# **Referred Books:**

- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Acheson, R.M. Introduction to the Chemistry of Heterocyclic compounds, John Welly& Sons (1976).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
- Kalsi, P. S. Textbook of Organic Chemistry 1st Ed., New Age International (P) Ltd. Pub.
- Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.
- Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, PrajatiParakashan (2010).

- Learn preparations, properties and chemical reactivity of nitrogen containing functional groups, polynuclear hydrocarbons, heterocyclic compounds and natural products.
- Understand the formation of carbon-hetero atom multiple bond.
- Isolation techniques of natural products and the classical methods of structural elucidation.

# Paper: Organic Chemistry – III Lab Paper Code: BCH-405

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

1.Functional group test for nitro, amine and amide groups.

2.Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols, carbonyl compounds and esters)

### **Referred Books:**

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

Paper: Physical Chemistry - IV Paper Code: BCH 403

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of conductance, chemical kinetics and cartalysis.

**Conductance:** Quantitative aspects of Faraday's laws of electrolysis Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at 29 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. (18 Lectures)

**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. (22 Lectures)

**Catalysis:** Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces. Enzyme catalysis, Michaelis-Menten mechanism, acid-base catalysis.(**8 Lectures**)

**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.

(12 Lectures)

**Referred Books:** 

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

- Strengthen the quantitative and practical aspect of electrolytic conductance.
- Understand the kinetics of various reactions.
- Understand the nature of catalyst and enzymes.
- Understand nature of biochemical and biophysical processes.

# Paper: Physical Chemistry – IV Lab Paper Code: BCH-406

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

# **Conductometry:**

- 1. Determination of cell constant.
- 2. Determination of conductivity, molar conductivity, degree of dissociation and dissociation constant of a weak acid.
- 3. 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.

# **Chemical Kinetics:**

Study the kinetics of the following reactions.

- 1. Iodide-persulphate reaction (i) Initial rate method; (ii)Integrated rate method
- 2. Acid hydrolysis of methyl acetate with hydrochloric acid.
- 3. Saponification of ethyl acetate.
- 4. Comparison of the strengths of HCl and H<sub>2</sub>SO<sub>4</sub> by studying kinetics of hydrolysis of methyl acetate.

# **Chemical Kinetics:Referred Books:**

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

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# SEMESTER V

#### Syllabus of B.Sc. (H) Chemistry

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Semester V

Paper: Organic Chemistry - IV Paper Code: BCH 501

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

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### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept synthesis, properties and chemical reactivity of nucleic acids, amino acids, peptides, proteins, enzymes and lipids.

#### **Nucleic Acids**

Components of nucleic acids, Nucleosides and nucleotides; Structure, synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine; Structure of polynucleotides (DNA and RNA). (12 Lectures)

#### **Amino Acids, Peptides and Proteins**

Amino acids, Peptides and their classification.

 $\alpha$ -Amino Acids - Synthesis, ionic properties and reactions. Zwitterions, pKa 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; primary, secondary and tertiary structures of proteins, Denaturation. (21 Lectures)

# 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, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance. (8 Lectures)

# 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. (10 Lectures)

# **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.

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

# (9 Lectures)

# **Referred Books:**

- Berg, J.M., Tymoczko, J.L. and Stryer, L. (2006) Biochemistry. VIth Edition. W.H. Freeman and Co.
- Nelson, D.L., Cox, M.M. and Lehninger, A.L. (2009) Principles of Biochemistry. IV Edition. W.H. Freeman and Co.
- 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.

- Learn synthesis, properties and chemical reactivity of nucleic acids.
- Understand synthesis, properties and chemical reactivity of amino acids, peptides and proteins.
- Understand synthesis, properties and chemical reactivity of enzymes.
- Understand synthesis, properties and chemical reactivity of lipids.

# Paper: Organic Chemistry – IV Lab Paper Code: BCH-503

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

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.

# **Referred Books:**

• Manual of Biochemistry Workshop, 2012, Department of Chemistry, University of Delhi.

• Arthur, I. V. Quantitative Organic Analysis, Pearson.

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Paper: Physical Chemistry - V Paper Code: BCH 502

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of quantum chemistry, chemical bonding and molecular spectroscopy.

**Quantum Chemistry:** Historical background, classical ideas of energy and particle trajectory, Blackbody radiation and Plank's hypothesis of quantization of energy, photoelectric effect, Line spectra of atoms, diffraction of electrons, wave particle duality. De Broglie's relation, Heisenberg's uncertainty principle.

Postulates of quantum mechanics, Concept and significance of wave function, quantum mechanical operators and commutation rules, (Linear, Hermitian, Laplacian and Hamiltonian operators), Schrödinger wave equation and its application to free particle and —particle-in-a-boxl (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle, probability distribution functions, nodal properties, expectation values, Extension to two and three dimensional boxes, separation of variables, degeneracy, Comparison of classical and quantum mechanics.

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

**Statistical Mechanics:** Ensemble averaging, postulates of ensemble averaging. Microcanonical, canonical and grand canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermind multipliers). Maxwell- Boltzmann statistics, Boltzmann distribution, derivation of the Boltzmann distribution expression, determination of the Boltzmann constant, Maxwell distribution law of velocities from Boltzmann distribution expression. Derivation of equation of states for a monoatomic ideal gas.

#### (30 Lectures)

**Molecular Spectroscopy:** Interaction of electromagnetic radiation with molecules and various types of spectra; Resolving power, width and intensity of spectral lines, broadening, signal to noise ration, 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 ( $\delta$  and T), spin-spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules.

# (30 Lectures)

# **Referred Books:**

- Benwell, Molecular spectroscopy
- Berg, J.M., Tymoczko, J.L. and Stryer, L. (2006) Biochemistry. VIth Edition. W.H. Freeman and Co.
- Nelson, D.L., Cox, M.M. and Lehninger, A.L. (2009) Principles of Biochemistry. IV Edition. W.H. Freeman and Co.
- 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.
- Kakkar, R. Atomic & Molecular Spectroscopy, Cambridge University Press (2015)

- Learn basic concept of quantum chemistry and qualitative treatment of vibrational motion.
- Understand theoretical aspects of s, p, d & f orbitalArrangement of electrons in atom.
- Concept of s, p, d and f orbitals and their shape using.
- Concepts of evaluation of various structural parameters using spectroscopic techniques.

# Paper: Physical Chemistry – V Lab Paper Code: BCH-504

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

# **Colorimetry :**

- I. Verify Lambert-Beer's law and determine the concentration of CuSO4/KMnO4/K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> in a solution of unknown concentration
- II. Determine the concentrations of KMnO4 and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> 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-phenathroline.
- V. Determine the dissociation constant of an indicator (phenolphthalein).
- VI. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

# **Spectroscopy:**

Analysis of the given vibration-rotation spectrum of HCl(g)

# UV/Visible spectroscopy:

I. Study the 200-500 nm absorbance spectra of KMnO4 and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> (in 0.1 M H<sub>2</sub>SO4) and determine the  $\lambda_{max}$  values. Calculate the energies of the two transitions in different units

 $(J \text{ molecule}^{-1}, kJ \text{ mol}^{-1}, cm^{-1}, eV).$ 

II. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

# **Referred Books:**

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

#### Syllabus of B.Sc. (H) Chemistry

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**Semester V – Discipline Elective Course** 

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Paper: Analytical Chemistry Paper Code: DECC 501

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the quantitative and qualitative analysis and different separation techniques.

#### Qualitative and quantitative aspects of analysis:

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution of indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals. (5 Lectures)

#### **Optical methods of analysis:**

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.

*UV-Visible Spectrometry:* Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;

*Basic principles of quantitative analysis:* estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers.

*Flame Atomic Absorption and Emission Spectrometry:* Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples. (25 Lectures)

#### Thermal methods of analysis:

Theory of thermogravimetry (TG), basic principle of instrumentation. Techniques for quantitative estimation of Ca and Mg from their mixture (Oxalate/carbonate).

(5 Lectures)

#### **Electroanalytical methods:**

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pKa values. (10 Lectures)

# Separation techniques:

Solvent extraction Classification, principle and efficiency of the technique. Mechanism of extraction: extraction by solvation and chelation. Technique of extraction: batch, continuous and counter current extractions.

Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and non-aqueous media.

Chromatography: Classification, principle and efficiency of the technique. Mechanism of separation: adsorption, partition & ion exchange. Development of chromatograms: frontal, elution and displacement methods. (15 Lectures)

# **Referred Books:**

- Vogel, Arthur I: A Text book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5<sup>th</sup> Ed. The English Language Book Society of Longman.
- Willard, Hobart H. et al.: *Instrumental Methods of Analysis*, 7<sup>th</sup> Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Christian, Gary D; Analytical Chemistry, 6<sup>th</sup> Ed. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age, International Publisher, 2009.
- Skoog, D.A., Holler F.J. and Nieman, T.A. *Principles of Instrumental Analysis*, Thomson Asia Pvt. Ltd. Singapore, 1998.
- Mikes, O. and Chalmers, R.A. Ed. *Laboratory Hand Book of Chromatographic and Allied Methods*, Elles Horwood Ltd. London.
- Dilts, R.V. Analytical Chemistry Methods of separation Van Nostrand 1974.

- Strategically analyze the given sample.
- Understand the principle, instrumentation and applications of spectroscopic methods.
- Concept of different separation techniques.
- Understand different thermal analytical methods.

# Paper: Analytical Chemistry Lab Paper Code: DECC-504

No. of Credits: 2 L: 0, T: 0, P: 2 60 Periods Internal: 15 External Exam: 35 Total: 50

# **Separation Techniques**

I Chromatography:

- Paper chromatographic separation of Co<sup>2+</sup> and Ni<sup>2+</sup>.
- Separation and identification of the amino acids present in the given mixture by paper chromatography. Reporting the Rf values.

II. Solvent Extractions:

• To separate a mixture of Ni & Fe by complexation with DMG and extracting the Ni<sup>2+</sup>.DMG complex in chloroform, and determine its concentration by spectrophotometry.<sup>2+2+</sup>

III Analysis of soil:

(i) Determination of pH of soil.

(ii) Total soluble salt

(iii) Estimation of calcium, magnesium

(iv) Qualitative detection of nitrate, phosphate

IV Ion exchange:

(i) Determination of exchange capacity of cation exchange resins and anion exchange resins.

(ii) Separation of amino acids from organic acids by ion exchange chromatography.

**III Spectrophotometry** 

Verification of Lambert-Beer's law and determination of concentration of a coloured species (CuSO<sub>4</sub>, KMnO<sub>4</sub>)

# **Referred Books:**

- Vogel, Arthur I: *A Text book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5<sup>th</sup> Ed. The English Language Book Society of Longman.
- Willard, Hobart H. et al.: *Instrumental Methods of Analysis*, 7<sup>th</sup> Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Christian, Gary D; Analytical Chemistry, 6<sup>th</sup> Ed. John Wiley & Sons, New York, 2004.

- Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age, International Publisher, 2009.
- Skoog, D.A. Holler F.J. and Nieman, T.A. *Principles of Instrumental Analysis*, Thomson Asia Pvt. Ltd. Singapore, 1998.
- Mikes, O. & Chalmers, R.A. *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Horwood Ltd. London.

Paper: Polymer Chemistry Paper Code: DECC 502

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

# **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept polymerization, crystallization and crystallinity.

# Introduction and history of polymeric materials:

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers. (4 Lectures)

# 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. (8 Lectures)

# **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. (8 lectures)

# **Crystallization and crystallinity:**

Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point. (4 Lectures)

Nature and structure of polymers-Structure Property relationships. (2 Lectures)

**Determination of molecular weight of polymers** (*Mn*, *Mw*, etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index. (8 Lectures)

**Glass transition temperature (Tg) and determination of Tg**, Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg). (8 Lectures)

**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. **(8 Lectures)** 

**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)]. (10 Lectures)

# **Referred Books:**

- Seymour's Polymer Chemistry, Marcel Dekker, Inc.
- G. Odian: Principles of Polymerization, John Wiley.
- F.W. Billmeyer: Text Book of Polymer Science, John Wiley.
- P. Ghosh: Polymer Science & Technology, Tata Mcgraw-Hill.
- R.W. Lenz: Organic Chemistry of Synthetic High Polymers.

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- Understand the introduction and history of polymers.
- Understand the kinetics and importance of polymerization.
- Determine the molecular weight of polymers, gas transition temperature and its determination.
- Have a brief idea about polymer solution and properties of polymers.

# Paper: Polymer Chemistry Lab Paper Code: DECC-505

No. of Credits: 2 L: 0, T: 0, P: 2 60 Periods Internal: 15 External Exam: 35 Total: 50

# **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-isobutylonitrile (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).

# **Polymer characterization**

Determination of molecular weight by viscometry:
 (a) Polyacrylamide-aq.NaNO2 solution

(b) (Poly vinyl proplylidine (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.

- 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.

# **Referred Books:**

- Malcohm P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
- Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)
- Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
- Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)
- Petr Munk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)
- L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)
- Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd ed. Oxford University Press (2005)
- Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013)..

# Paper: Cement Chemistry Paper Code: DECC 503

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

To study about chemical aspects of cement manufacture. To learn about chemistry of clinker and cement formation, hydration reactions of cement, types of cement and quality control measures for cement manufacture.

**Raw Materials and Cement Manufacture:** History of cement, Indian cement industry. Raw materials – calcareous and argillaceous materials, corrective materials and usage of industrial wastes as cement raw materials. Process of cement manufacture, Overview of various unit operations in cement manufacture.

# (15 Lectures)

**Raw Mix Design and Clinker Formation:** Raw mix proportioning and composition, Modulii values and their significance, Raw mix design for 2, 3, 4 – component raw mix. Burnability of raw mix, effect of various factors on burnability of raw mix, absorption and effect of coal ash. Chemical and phase composition of clinker, Chemical reactions during clinkerization, Bogue calculation. Fuels, Mineralizer and Fluxes. (15 Lectures)

**Cement Hydration**: Hydration of cement, Setting, hardening and strength development. Role of various clinker phases on cement performance. Use of waste materials – fly ash, slag, Pozzolanic reaction, Hydration of slag. (15 Lectures)

**Types of Cement and Quality Control:** BIS specifications and use of various types of cement with emphasis on Ordinary Portland Cement (OPC – 33 grade, 43 grade and 53 grade), Portland Pozzolana Cement (PPC) and Portland Slag Cement (PSC). Quality control in cement manufacture. Physical and chemical testing of cement. (15 Lectures)

Course Outcomes: After the successful completion of the course the learner would be able to

- Design suitable raw mix for clinker/ cement manufacture.
- Carry out physical and chemical testing of cement.
- Monitor and control quality of cement during process of cement manufacture.

**Reference Books:** 

- 1. Cement Chemistry. H.F.W.Taylor, 3<sup>rd</sup> Edn. Academic Press, London
- 2. Chemistry of Cement and Concrete, F.M.Lea, 4th Edn. Arnold, London
- 3. Cement Data Book. Vol.1 W.H.Duda, Verlag Gm Bh., Berlin
- 4. Cement Enginners' Handbook, Labhan and Kolhaans
- 5. Advances in Cement Technology, S.N.Ghosh, 2<sup>nd</sup> Edn., CRC Press
- 6. NCB Guide Norms for Cement Plant Operation, National Council for Cement and Building Materials Publication

Bureau of Indian Standards Specifications IS: 4031 and 4032

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# Paper: Cement Chemistry Lab Paper Code: DECC-506

No. of Credits: 2 L: 0, T: 0, P: 2 60 Periods Internal: 15 External Exam: 35 Total: 50

# Physical and Chemical Testing (BIS Specifications IS: 4031 and 4032)

# (A) Sieve Analysis

- (i) Sieve Analysis of Clincker
- (ii) Sieve Analysis of Cement on 90  $\mu$  and 45  $\mu$  sieve

# **(B)** Specific Gravity Determination

- (i) Determination of specific gravity of Ordinary Portland Cement (OPC)
- (ii) Determination of specific gravity of Portland Pozzolana Cement (PPC)
- (iii)Determination of specific gravity of Portland Slag Cement (PSC)

# (C) Fineness Determination

- (i) Determination of Fineness of Ordinary Portland Cement (OPC)
- (ii) Determination of Fineness of Ordinary Portland Cement (OPC)
- (iii)Determination of Fineness of Ordinary Portland Cement (OPC)

# **(D)** Chemical Analysis

- (i) Chemical analysis of Cement
- (ii) Chemical analysis of Clinker
- (iii)Chemical analysis of Flyash
- (iv)Chemical analysis of Limestone

# **Referred Books:**

Vogel, A.I. A Textbook of Quantitative Inorganic Analysis, ELBS.

# SEMESTER VI

**Semester VI** 

# Paper: Inorganic Chemistry - IV Paper Code: BCH 601

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

# **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of qualitative analysis, organometallic chemistry and bio-inorganic chemistry.

# **Theoretical Principles in Qualitative Analysis**

Basic principles involved in analysis of cations and anions. 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. (12 Lectures)

# **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.  $\pi$ -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.

Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene. (26 Lectures)

# **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, Cisplatin as an anti-cancer drug.

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

(14 Lectures)

# **Catalysis by Organometallic Compounds**

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinson's Catalyst)

2. Synthetic gasoline (Fischer Tropsch reaction)

3. Polymerisation of ethene using Ziegler-Natta catalyst Referred Books:

(8 Lectures)

- Svehla, G. Vogel's Qualitative Inorganic Analysis, 7th Edition, Prentice Hall, 1996-03-07.
- Lippard, S.J. & Berg, J.M., *Principles of Bioinorganic Chemistry* Panima Publishing Company 1994.
- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of
- Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005
- Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry3<sup>rd</sup> Ed.*, John Wiley and Sons, NY, 1994.
- Greenwood, N.N. & Earnshaw, A. *Chemistry of the Elements 2<sup>nd</sup> Ed*, Elsevier, 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
- Lee, J.D. *Concise Inorganic Chemistry* 5<sup>th</sup> Ed., John Wiley and sons 2008.
- Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988.
- Shriver, D.D., Atkins, P. and Langford, C.H., *Inorganic Chemistry* 2<sup>nd</sup> Ed., Oxford University Press, 1994.

- Understand the basic principles of the analysis of cations and anions.
- Learn general chemistry of organometallic compounds.
- Learn basic concepts of bio-inorganic chemistry.
- Understand catalytic activity of organometallic compounds.

#### Paper: Inorganic Chemistry – IV Lab Paper Code: BCH-603

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

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:

 $CO_3^{2^-}$ ,  $NO_2^{-}$ ,  $S^{2^-}$ ,  $SO_3^{2^-}$ ,  $S_2O_3^{2^-}$ ,  $CH_3COO^-$ ,  $F^-$ ,  $CI^-$ ,  $Br^-$ ,  $I^-$ ,  $NO_3^-$ ,  $BO_3^{3^-}$ ,  $C_2O_4^{2^-}$ ,  $PO_4^{3^-}$ ,  $NH_4^+$ ,  $Pb^{2^+}$ ,  $Cu^{2^+}$ ,  $Cd^{2^+}$ ,  $Bi^{3^+}$ ,  $Sn^{2^+}$ ,  $Sb^{3^+}$ ,  $Fe^{3^+}$ ,  $Al^{3^+}$ ,  $Cr^{3^+}$ ,  $Zn^{2^+}$ ,  $Mn^{2^+}$ ,  $Co^{2^+}$ ,  $Ni^{2^+}$ ,  $Ba^{2^+}$ ,  $Sr^{2^+}$ ,  $Ca^{2^+}$ ,  $Mg^{2^+}$ 

Mixtures should preferably contain one interfering anion, **or** insoluble component (BaSO<sub>4</sub>, SrSO<sub>4</sub>, PbSO<sub>4</sub>, CaF<sub>2</sub> or Al<sub>2</sub>O<sub>3</sub>) **or** combination of anions e.g.  $CO_3^2$  and  $SO_3^2$ , NO<sub>2</sub> and NO<sub>3</sub>, Cl and Br , Cl and I , Br and I , NO<sub>3</sub> and Br , NO<sub>3</sub> and I .

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

- Ni (II) and Co (II)
- Cu(II) and Cd(II)

# **Referred Books:**

- Vogel's Qualitative Inorganic Analysis, Revised by G. Svehla.
- Vogel, A.I. A Textbook of Quantitative Analysis, ELBS. 1986

Semester VI

# Paper: Organic Chemistry - V Paper Code: BCH 602

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

# **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept organic spectroscopy and some important organic compounds viz. carbohydrates, dyes and polymers.

#### **Organic Spectroscopy**

General principles Introduction to absorption and emission spectroscopy.

*UV Spectroscopy*: Types of electronic transitions,  $\lambda_{max}$ , Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of  $\lambda$ max for the following systems:  $\alpha$ , $\beta$ -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, Interpetation of NMR spectra of simple compounds.

Applications of IR, UV and NMR for identification of simple organic molecules. (24 Lectures)

#### 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. (16 Lectures)

# Dyes

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

Synthesis and applications of: Azo dyes – Methyl orange; Triphenyl methane dyes - Malachite green and Rosaniline ; Phthalein Dyes – Phenolphthalein; Natural dyes – structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes with examples. **(8 Lectures)** 

# Polymers

Introduction and classification including di-block, tri-block and amphiphilic polymers;

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; Biodegradable and conducting polymers with examples. (12 Lectures)

Referred Books:

- Kalsi, P. S. Textbook of Organic Chemistry 1st Ed., New Age International (P) Ltd. Pub.
- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Billmeyer, F. W. Textbook of Polymer Science, John Wiley & Sons, Inc.
- Gowariker, V. R.; Viswanathan, N. V. &Sreedhar, J. Polymer Science, New Age International (P) Ltd. Pub.
- Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.

- Learn basic concept of Spectroscopy and its applications in structural elucidation of organic compounds.
- Understand principles of UV, IR and NMR spectroscopy and their detailed study.
- Understand carbohydrate chemistry.
- Chemistry of dyes and polymers and their applications.

# Paper: Organic Chemistry – V Lab Paper Code: BCH-103

No. of Credits: 2 L: 0, T: 0, P: 4 60 Periods Internal: 15 External Exam: 35 Total: 50

1.Extraction of caffeine from tea leaves.

2. Preparation of urea formaldehyde resin.

- 3.Qualitative analysis of unknown organic compounds containing monofunctional groups (carbohydrates, aryl halides, aromatic hydrocarbons, nitro compounds, amines and amides) and simple bifunctional groups, e.g. salicylic acid, cinnamic acid, nitrophenols etc.
- 4.Identification of simple organic compounds by IR spectroscopy and NMR spectroscopy (Spectra to be provided).

5. Preparation of methyl orange.

# **Referred Books:**

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

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#### Syllabus of B.Sc. (H) Chemistry

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#### **Semester VI – Discipline Elective Course**

Paper: Medicinal Chemistry Paper Code: DECC 601

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of drug design and drug action and medicinal chemistry.

Introduction to medicinal chemistry, history and development of medicines. Concept of drug design and drug development, lead compound and lead modification, prodrugs and soft drugs, an elementary idea of structure reactivity relationship (SAR), Elementary idea about drug action: Drug receptor interactions and theories of drug action, neurotransmitters and receptors, ion channels and their control, membrane bound enzymes-activation/deactivation, chemical basis of messenger induced change of shape by the receptor. Physicochemical and stereochemical aspects of drug action Solubility, Drug absorption, surface area and particle size, hydrogen bonding and biological activity, polymorphism, stereochemistry and pharmacological activity. (**35 Lectures**)

Definition, uses and side effects of the following categories of drugs:

Antipyretics, analgesics & anti-inflammatory agents (paracetamol, asprin, mefenamic acid, ibuprofen and diclofenac), antimalarial (Chloroquine, chloroguanide), Anticancer (Chlorambucil, cyclophosphamide), Cardiovascular drugs (sorbitrate, diltiazem), Antifertility agents (introduction to hormonal and nonhormonal contraception only). (25 Lectures)

# **Referred Books:**

- Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Ed. Robert F. Dorge.
- Burger's Medicinal Chemistry and Drug Discovery, Vol-I, Ed. M.E.Wolf, John Wiley.
- Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.

- Learn basic concept of medicinal chemistry. Drug design and drug development. Synthesis and uses of some important drugs. •
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# Paper: Medicinal Chemistry Lab Paper Code: DECC-604

No. of Credits: 2 L: 0, T: 0, P: 2 30 Periods Internal: 15 External Exam: 35 Total: 50

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of drug design and drug action and medicinal chemistry.

- 1. Quantitative estimation of Quinine in Cinchona bark by HPLC method.
- 2. Exercises on Identification of simple Naturally occurring molecules by UV, IR and NMR spectroscopy.
- 3. Extraction and isolation of pectin, starch, caffeine, piperine, solanine, aromatic oils, calcium citrate, solanine, casein, etc.
- 4. Synthesis and characterization of biologically active hetero-cyclic nuclei such as hydantoin, indole, furan, benzofuran, benimidazole etc.

# **Referred Books:**

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

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# Paper: Molecular Modeling & Drug Design Paper Code: DECC 602

No. of Credits: 4 L: 4, T: 0 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of molecular modeling and drug design.

#### **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. (10 Lectures)

#### **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. (14 Lectures)

# **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. (12 Lectures)

#### 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. (12 Lectures)

#### **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. (12 Lectures)

#### **Referred Books:**

• A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.

- J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
- Satya Prakash Gupta, QSAR and Molecular Modeling, Springer Anamaya Publishers, 2008.

- Learn the basics of molecular modeling.
- Understand the concept of force fields, energy minimization and computer simulation.
- Understand the concept of molecular dynamics and monte calo simulation.
- Understand the concept of structure prediction and drug design.

# Paper: Molecular Modeling & Drug Design Lab Paper Code: DECC-605

No. of Credits: 2 L: 0, T: 0, P: 2 30 Periods Internal: 15 External Exam: 35 Total: 50

i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane  $\zeta$  bonds and ethene, ethyne, benzene and pyridine  $\pi$  bonds.

ii. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.

iii. 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.

iv. (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.

v. (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).

vi. 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.

vii. (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.

viii. 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.

ix. (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.

# **Referred Books:**

- A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
- J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
- Satya Prakash Gupta, QSAR and Molecular Modeling, Springer Anamaya Publishers, 2008

# Paper: Research Methodology for Chemistry Paper Code: DECC 603

No. of Credits: 6 L: 5, T: 1 Theory: 60 Lectures Sessional: 25 Theory Exam: 75 Total: 100

#### **COURSE OBJECTIVE**

The objective of the course is to make the students understand the basic concept of research, literature survey, chemical safety and ethical handling of chemicals, data analysis and scientific research paper writing.

#### 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. (20 Lectures)

# 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. (20 Lectures)

#### **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. (12 Lectures)

# **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. (13 Lectures)

# 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. (10 Lectures)

# **Referred Books:**

- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) *Practical skills in chemistry*. 2nd Ed. Prentice-Hall, Harlow.
- Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
- Topping, J. (1984) *Errors of observation and their treatment*. Fourth Ed., Chapman Hall, London.
- Harris, D. C. *Quantitative chemical analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis.* Cambridge Univ. Press (2001) 487 pages.
- Chemical safety matters IUPAC IPCS, Cambridge University Press, 1992.
- OSU safety manual 1.01.

- Do literature survey of the topic of research.
- Learn how to write a scientific article.
- Handle the chemicals in lab and perform safe experiments.
- Understand data analysis.