

# **CHOICE BASED CREDIT SYSTEM (CBCS)**

## **Syllabus for Chemistry**

**B. Sc.**

**(HONOURS & GENERIC ELECTIVE)**



इन्दिरा गांधी राष्ट्रीय जनजातीय विश्वविद्यालय  
Indira Gandhi National Tribal University

अमरकंटक (म.प्र.) | Amarkantak (M.P.)

(भारतीय संसद में पारित अधिनियम द्वारा स्थापित केन्द्रीय विश्वविद्यालय)  
(A Central University Established by an Act of Parliament of India)








## ABOUT THE DEPARTMENT

### Department of Chemistry, IGNTU, Amarkantak

The Department of Chemistry was started in 2008, and has now grown into a major department for teaching and research within the Faculty of Science at IGNTU. The department offer vibrant atmosphere to students and faculty to encourage the spirit of scientific inquiry and to pursue cutting-edge research in a highly encouraging environment. The key objective of our department is to create good quality human resource through competitive yet inspiring environment for developing their careers. Currently, the department comprises more than hundred students, five research scholar and seven faculties and a dedicate team of staff members. The department offers three years undergraduate B.Sc. courses in Chemistry (Hons.) in the University. In addition it also offers two years M. Sc. and PhD programme. At present the Department consists of about seven research groups working in the areas of material chemistry (Functional Hybrid Nanomaterials), coordination/supramolecular chemistry, bioinorganic chemistry, asymmetric synthesis, catalysis, nanomagnetism and Single Molecule Magnets (SMMs), as major thrust areas. The department is doing well in research activities and published good numbers of research papers. The faculty has been undertaking research projects sponsored by different national agencies such as DST, UGC, etc. The most important achievement of the University is the first Department of Chemistry has succeeded “**DST-FIST Program – 2017**” recognition from Govt. of India, Department of Science & Technology, New Delhi. Many students have been qualified National Eligibility Test (NET) and Joint Admission Test (JAM) Examination for pursuing PhD and M. Sc. Program in different prestigious IIT, NIT and Central Universities. The most of the students of our department is tribal and our mission is that the department of Chemistry can be reached at highest level in the country for its teaching and research activities and produced number of best quality of students in India.

## At a Glance Department of Chemistry, IGNTU

### Faculty Profile

Presentation	Name & Designation	Research Area	Awards and Honors
	<b>Dr. Tanmay K Ghorai</b> Associate Professor & Head <i>PhD: IIT-KGP</i>	Nanoscience, Catalysis & Single Molecule Magnets	BOYSCAST Fellowship & Young Scientist Award (DST)
	<b>Dr. Subrata Jana</b> Associate Professor <i>PhD: IEST-Shibpur</i>	Molecular Recognition & Supramolecular Chemistry	Radhika Panda Memorial Award, UrFU PDF Award
	<b>Dr. Khemchand Dewangan</b> Assistant Professor <i>PhD: IIT-Kanpur</i>	Nanostructure Transition Metal Oxides & Nitrides	BSR-UGC Start-Up Grant
	<b>Dr. Adhish Jaiswal</b> Assistant Professor <i>PhD: NCL-Pune</i>	Dielectrics, Magnetism & Solar- cell	Best Research Scholar Award in NCL Pune
	<b>Dr. Biswajit Maji</b> Assistant Professor <i>PhD: IIT-KGP</i>	Asymmetric Synthesis and Catalysis	INSPIRE Faculty Award, President INSPIRE Teacher Recognition
	<b>Dr. Sadhu Charan Mallick</b> Assistant Professor <i>PhD: IITGuwahati</i>	Metal Nano Particles, Polymer Composites & Bio applications	Best Poster Award at ICT Hyderabad
	<b>Dr. Ajay Shankar</b> Assistant Professor <i>PhD: NPL, Delhi</i>	Nano- magnetism	Post- Doctoral fellowship Award at Germany

**Members of the Board of Studies**


**For**

**Revised the Chemistry Syllabus of  
B. Sc. (HONOURS & GENERIC ELECTIVE)**


**According**

**CHOICE BASED CREDIT SYSTEM  
(CBCS)**


The syllabus of B.Sc. (Hon's & Generic Elective Course for other Department) is hereby approved in a meeting of the members of the Board of Study for the Department of Chemistry, Indira Gandhi National Tribal University, Amarkantak (M.P.) on February 6, 2017, Monday.



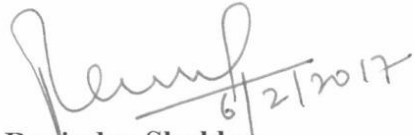
**Prof. Ashish K. Prajapati**  
Professor  
(Member, External Expert)  
Department of Chemistry,  
The M. S. University of Baroda




**Dr. Raghumani Singh Ningthoujam**  
Scientist-E  
(Member, Special Invitee)  
Chemistry Division  
Bhabha Atomic Research Centre




**Dr. Tarun Thakur**  
Associate Professor  
(Member)  
Department of Environmental Science  
IGNTU



**Dr. Ravindra Shukla**  
Assistant Professor  
(Member)  
Department of Botany  
IGNTU



**Dr. Subrata Jana**  
Associate Professor  
(Member)  
Department of Chemistry  
IGNTU



**Dr. Tanmay Kumar Ghorai**  
Associate Professor & Head  
(Chairman)  
Department of Chemistry  
IGNTU

# Course Structure (Chemistry-Major)

## Details of courses under B.Sc. (Honours)

Course	*Credits	
	Theory+ Practical	Theory + Tutorial
=====		
<b>I. Core Course</b>		
<b>(14 Papers)</b>	14×4= 56	14×5=70
<b>Core Course Practical / Tutorial*</b>		
<b>(14 Papers)</b>	14×2=28	14×1=14
<b>II. Elective Course</b>		
<b>(8 Papers)</b>		
A.1. Discipline Specific Elective	4×4=16	4×5=20
<b>(4 Papers)</b>		
A.2. Discipline Specific Elective		
Practical/Tutorial*	4×2=8	4×1=4
<b>(4 Papers)</b>		
B.1. Generic Elective/		
Interdisciplinary	4×4=16	4×5=20
<b>(4 Papers)</b>		
B.2. Generic Elective		
Practical/ Tutorial*	4×2=8	4×1=4
<b>(4 Papers)</b>		
<input type="checkbox"/> <b>Optional Dissertation or project work in place of one Discipline Specific Elective paper (6 credits) in 6<sup>th</sup> Semester</b>		
<b>III. Ability Enhancement Courses</b>		
<b>1. Ability Enhancement Compulsory</b>		
<b>(2 Papers of 4 credit each)</b>	2×4=8	2×4=8
Environmental Science		
English/MIL Communication		
<b>2. Ability Enhancement Elective (Skill Based)</b>		
<b>(Minimum 2)</b>	2×4=8	2×4=8
<b>(2 Papers of 4 credit each)</b>		
<b>Total credit</b>	<b>148</b>	<b>148</b>

\* wherever there is a practical there will be no tutorial and vice-versa

## **PROPOSED SCHEME FOR CHOICE BASED CREDIT SYSTEM IN**

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

SEM	CORE COURSE (14)	Ability Enhancement Compulsory Course (AECC) (2)	Ability Enhancement Elective Course (AEEC) (2) (Skill Based)	Elective: Discipline Specific DSE (4)	Elective: Generic (GE) (4)
I	Inorganic I: Atomic Structure & Chemical Bonding-I (4+2)	(English Communication/MIL) /Environmental Science			GE – I
	Physical I: States of Matter & Ionic Equilibrium (4+2)				
II	Organic I: Basics & Hydrocarbons (4+2)	(English Communication/MIL) /Environmental Science			GE – II
	Physical II: Chemical Thermodynamics & Chemical Equilibrium (4+2)				
III	Inorganic II: Radioactivity & s- and p-Block Elements (4+2)		SEC – I		GE – III
	Organic II: Oxygen Containing Functional Groups (4+2)				
	Physical III: Phase Equilibria, Solution & Chemical Kinetics (4+2)				
IV	Inorganic III: Coordination Chemistry (4+2)		SEC – II		GE – IV
	Organic III: Heterocyclic Chemistry (4+2)				
	Physical IV: Catalysis, Electro and Photo-Chemistry (4+2)				
V	Organic IV: Biomolecules (4+2)			DSE – I	
	Physical V: Quantum Chemistry & Spectroscopy (4+2)			DSE – II	
VI	Inorganic IV: Organometallic Chemistry (4+2)			DSE – III	
	Organic V: Spectroscopy (4+2)			DSE – IV	

<b>Course Structure for B.Sc.</b>			
<b>CHEMISTRY HONORS</b>			
<i>1 credit = 1 hour per week for Theory and 2 hours per week for Laboratory</i>			
<b>Course Code</b>	<b>Course Structure</b>	<b>Course Name</b>	<b>Credit</b>
<b>SEMESTER-I</b>			
	Ability Enhancement Compulsory Course – I	English Communications/Environmental Science (offered by respective Department)	4
CHM T 111	Core Course – I	Inorganic Chemistry I: Atomic Structure & Chemical Bonding	4
CHM P 111	Core Course – I Practical	Inorganic Chemistry - I Lab	2
CHMT 112	Core Course-II	Physical Chemistry I: States of Matter & Ionic Equilibrium	4
CHM P 112	Core Course – I Practical	Physical Chemistry - I Lab	2
CHM T 113 ***GE - (A-G)	Generic Elective – I	GE - I (Opted subject from Table GE offered by Department)	4
CHM P 113 ***GE - (A-G)	Generic Elective – I Practical	GE Chemistry Practical – I Lab	2
<b>SEMESTER-II</b>			
	Ability Enhancement Compulsory Course – II	English Communications/Environmental Science (offered by respective Department)	4
CHM T 121	Core Course – III	Organic Chemistry – I: Basics and Hydrocarbons	4
CHM P 121	Core Course – III Practical	Organic Chemistry – I Lab	2
CHM T 122	Core Course – IV	Physical Chemistry – II: Chemical Thermodynamics and Chemical Equilibrium	4
CHM P 122	Core Course – IV Practical	Physical Chemistry – II Lab	2
CHM T 123 ***GE - (A-G)	Generic Elective – II	GE - II (Opted subject from Table GE offered by Department)	4
CHM P 123 ***GE - (A-G)	Generic Elective – II Practical	GE Chemistry Practical – II Lab	2
<b>SEMESTER-III</b>			
CHM T 211	Core Course – V	Inorganic Chemistry – II : Radioactivity & s- and p-Block Elements	4
CHM P 211	Core Course – V Practical	Inorganic Chemistry – II Lab	2
CHM T 212	Core Course – VI	Organic Chemistry – II: Oxygen Containing Functional Groups	4
CHM P 212	Core Course – VI Practical	Organic Chemistry – II Lab	2
CHM T 213	Core Course – VII	Physical Chemistry – III: Phase Equilibria, Solution and Chemical Kinetics	4
CHM P 213	Core Course – VII Practical	Physical Chemistry – III Lab	2
CHM T 214 **SEC - (A-H)	Skill Enhancement Course – I	SEC-I (Opted subject from Table SEC offered by Department)	4
CHM T 215 ***GE - (A-G)	Generic Elective – III	GE - III (Opted subject from Table GE offered by Department)	4

CHM P 215 ***GE - (A-G)	Generic Elective – III Practical	GE Chemistry Practical – III Lab	2
<b>SEMESTER-IV</b>			
CHM T 221	Core Course – VIII	Inorganic Chemistry III: Coordination Chemistry	4
CHM P 221	Core Course – VIII Practical	Inorganic Chemistry – III Lab	2
CHM T 222	Core Course – IX	Organic Chemistry – III: Introduction of N – Containing Functional Group Towards Heterocyclic Chemistry	4
CHM P 222	Core Course – IX Practical	Organic Chemistry – III Lab	2
CHM T 223	Core Course – X	Physical Chemistry – IV: Catalysis, Electro and Photo-Chemistry	4
CHM P 223	Core Course – X Practical	Physical Chemistry – IV Lab	2
CHM T 224 **SEC - (A-H)	Skill Enhancement Course – II	SEC-II (Opted subject from Table SEC offered by Department)	4
CHM T 225 ***GE - (A-G)	Generic Elective – IV	GE – IV (Opted subject from Table GE offered by Department)	4
CHM P 225 ***GE - (A-G)	Generic Elective – IV Practical	GE Chemistry Practical –IV Lab	2
<b>SEMESTER-V</b>			
CHM T 311	Core Course – XI	Organic Chemistry – IV: Biomolecules	4
CHM P 311	Core Course – XI Practical	Organic Chemistry – IV Lab	2
CHM T 312	Core Course – XII	Physical Chemistry – V: Quantum Chemistry & Spectroscopy	4
CHM P 312	Core Course – IX Practical	Physical Chemistry – V Lab	2
CHM T 313 *DSE - (A - M)	Discipline Specific Elective – I	DSE – I (Opted subject from Table DSE offered by Department)	4
CHM P 313 *DSE - (A - M)	Discipline Specific Elective – I Practical	DSE – I Lab	2
CHM T 314 *DSE - (A - M)	Discipline Specific Elective – II	DSE – II (Opted subject from Table DSE offered by Department)	4
CHM P 314 *DSE - (A - M)	Discipline Specific Elective – II Practical	DSE – II Lab	2
<b>SEMESTER-VI</b>			
CHM T 321	Core Course – XIII	Inorganic Chemistry – IV: Organometallic Chemistry	4
CHM P 321	Core Course – XIII Practical	Inorganic Chemistry – IV Lab	2
CHM T 322	Core Course – XIV	Organic Chemistry – V: Spectroscopy	4
CHM P 322	Core Course – XIV Practical	Organic Chemistry – V Lab	2
CHM T 323 *DSE - (A - M)	Discipline Specific Elective – III	DSE – III (Opted subject from Table DSE offered by Department)	4
CHM P 323 *DSE - (A - M)	Discipline Specific Elective – III Practical	DSE – III Lab	2
CHM T 324	Discipline Specific	DSE – IV (Opted subject from Table DSE	4

*DSE - (A - M)	Elective – IV	offered by Department)	
CHM P 324 *DSE - (A - L)	Discipline Specific Elective – IV Practical	DSE – IV Lab	2
<b>Grand Total</b>			<b>148</b>

\* Discipline Specific Elective (A – M) referred in Table DSE

\*\*Skill Enhancement Course (A – H) referred in Table SEC

\*\*\* General Elective Course (A – G) referred in Table GE

## Core Courses: (Credit: 06 each)

(1 period/week for tutorials or 4 periods/week for practical)

1. Inorganic Chemistry – I : Atomic Structure & Chemical Bonding (4 + 2)
2. Physical Chemistry – I : States of Matter & Ionic Equilibrium (4 + 2)
3. Organic Chemistry – I : Basics and Hydrocarbons (4 + 2)
4. Physical Chemistry – II : Chemical Thermodynamics and (4 + 2)
5. Inorganic Chemistry – II : Radioactivity & s- and p-Block Elements (4 + 2)
6. Organic Chemistry – II : Oxygen Containing Functional Groups (4 + 2)
7. Physical Chemistry – III : Phase Equilibria, Solution and Chemical Kinetics (4+2)
8. Inorganic Chemistry – III : Coordination Chemistry (4 + 2)
9. Organic Chemistry – III : Heterocyclic Chemistry (4 + 2)
10. Physical Chemistry – IV : Catalysis, Electro and Photo-chemistry (4 + 2)
11. Organic Chemistry – IV : Biomolecules (4 + 2)
12. Physical Chemistry – V : Quantum Chemistry & Spectroscopy (4 + 2)
13. Inorganic Chemistry – IV : Organometallic Chemistry (4 +2)
14. Organic Chemistry – V : Spectroscopy (4 + 2)

**Table DSE**

<b>*Discipline Specific Elective (DSE)</b>		
<b>Course Code</b>	<b>Title of Paper</b>	<b>Credit</b>
DSE – A	Applications of Computers in Chemistry	4
DSE – B	Analytical Methods in Chemistry	4
DSE – C	Basics of Drug Design & Medicinal Chemistry	4
DSE – D	Novel Inorganic Solids	4
DSE – E	Polymer Chemistry	4
DSE – F	Green Chemistry	4
DSE – G	Industrial Chemicals & Environment	4
DSE – H	Inorganic Materials of Industrial Importance	4
DSE – I	Instrumental Methods of Chemical Analysis	4
DSE – J	Basic of Nanomaterials	4
DSE – K	Advanced Organic Chemistry	4
DSE – L	Research Methodology for Chemistry	5 + 1(Tutorial)
DSE – M	Crystalline Material and Properties	5 + 1(Tutorial)
DSE – N	Basic Mathematical Concept for Chemist	5+1(Tutorial)

**Table SEC**

<b>**Skill Enhancement Course (SEC)</b>		
<b>Course Code</b>	<b>Title of Paper</b>	<b>Credit</b>
SEC – A	IT Skills for Chemists	4
SEC – B	Basic Analytical Chemistry	4
SEC – C	Chemical Technology & Environmental Aspects for Society	4
SEC – D	Chemoinformatics	4
SEC – E	Green Methods in Chemistry	4
SEC – F	Cosmetics, Perfumes & Pharmaceutical Chemistry	4
SEC – G	Pesticide & Fuel Chemistry	4
SEC – H	Computer Science/Sports/NCC/NSS/Yoga etc. offered by respective Department	4

**Table GE**

<b>*Generic Elective Course (GE)</b>		
<b>Course Code</b>	<b>Title of Paper</b>	<b>Credit</b>
GE – A	Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons	4
GE – B	Kinetic Theory of Gases, Chemical Energetics, Equilibria & Functional Group Organic Chemistry	4
GE – C	Solutions, Phase Equilibrium, Conductance and Chemistry of s-, p- and d- block elements	4
GE – D	Electrochemistry, Chemical Kinetics, Co-ordination compounds, Organometallics and Molecules of life	4
GE – E	Analytical Chemistry, Quantum Chemistry and Spectroscopy	4
GE – F	Chemistry of f-block elements, Bioinorganic Chemistry, Polynuclear hydrocarbons and UV, IR Spectroscopy	4
GE – G	Polymer Chemistry, Nuclear and Materials Chemistry	4

## SEMESTER – I

### CHM T 111: Inorganic Chemistry– I: Atomic Structure & Chemical Bonding

(Credits: Theory - 04, Practical - 02)

Theory: 60 Hours

#### Unit –1: Atomic Structure

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of  $\psi$  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. Contour boundary and probability diagrams.

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

(14 Hours)

#### Unit – 2: Periodicity of Elements

*s*, *p*, *d*, *f* block elements, the long form of periodic table. Detailed discussion of the following properties of the elements, with reference to *s* & *p*-block.

(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.

(b) Atomic radii (van der Waals)

(c) Ionic and crystal radii.

(d) Covalent radii (octahedral and tetrahedral)

(e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy.

(f) Electron gain enthalpy, trends of electron gain enthalpy.

(g) Electronegativity, Pauling's/ Mulliken's/ Allred Rachow's/ and Mulliken-Jaffé's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. Sanderson's electron density ratio.

(14 Hours)

#### Unit – 3: Chemical Bonding

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

(ii) *Covalent bond*: Lewis structure, Valence Bond theory (Heitler-London approach). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding ( $\sigma$  and  $\pi$  bond approach) and bond lengths. Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital

theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules  $N_2$ ,  $O_2$ ,  $C_2$ ,  $B_2$ ,  $F_2$ ,  $CO$ ,  $NO$ , and their ions;  $HCl$ ,  $BeF_2$ ,  $CO_2$ , (idea of s-p mixing and orbital interaction to be given).

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.

Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

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

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

**(20 Hours)**

#### **Unit – 4: Non-aqueous solvents**

Physical properties of a solvent, types of solvents and their general characteristics, reactions in non-aqueous solvents with reference to liquid  $NH_3$ , liquid  $SO_2$  and liquid  $HF$ .

**(4 Hours)**

#### **Unit – 5: Oxidation-Reduction**

Redox equations, Standard electrode potentials, redox potentials and formal potentials, Nernst equation, redox potentials to explore the feasibility of reaction and calculation of values of equilibrium constant, redox potential as a function of pH, precipitation and complex formation, redox titrations and redox indicators, Frost and Latimer diagrams of redox potentials.

**(8 Hours)**

#### **Reference Books:**

- Lee, J.D. Concise Inorganic Chemistry, ELBS, 1991.
- Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, Oxford, 1970
- Atkins, P.W. & Paula, J. Physical Chemistry, Oxford Press, 2006.
- Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications 1962.
- Wahid U. Malic, G. D. Tuli, R. D. Madan, Inorganic Chemistry, S. Chand & Co. Ltd
- R. Sarkar and N. Saha, General & Inorganic Chemistry, New Central Book Agency
- Puri, Sharma and Kalia, Principle of Inorganic Chemistry, Milestone publishers & distributors

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#### **CHM P 111: Inorganic Chemistry – I Lab:**

**(60 Hours)**

##### **(A) Titrimetric Analysis**

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

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

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

### **(C) Oxidation-Reduction Titrimetry**

- (i) Estimation of Fe(II) and oxalic acid using standardized  $\text{KMnO}_4$  solution.
- (ii) Estimation of oxalic acid and sodium oxalate in a given mixture.
- (iii) Estimation of Fe(II) with  $\text{K}_2\text{Cr}_2\text{O}_7$  using internal (diphenylamine, anthranilic acid) and external indicator.

### **Reference text:**

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

## **CHM T 112: Physical Chemistry- I: States of Matter & Ionic Equilibrium**

**(Credits: Theory-04, Practical-02)**

**Theory: 60 Hours**

### **Unit – 1: Gaseous State – I**

Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equations; deduction of gas laws from kinetic gas equation.

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

**(9 Hours)**

### **Unit – 2: Gaseous State – II**

Maxwell Boltzmann distribution laws of molecular velocity and molecular energies (graphic representation – derivation not required) 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.

Collision frequency, collision diameter, and mean free path including their temperature and pressure dependence; viscosity of gases, relation between mean free path and coefficient of viscosity; calculation of collision diameter from coefficient of viscosity; variation of viscosity with temperature and pressure.

**(9 Hours)**

### Unit – 3: Liquid State

Qualitative treatment of the structure of the liquid state; Radial distribution function; physical properties of liquids; vapor pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases. Qualitative discussion of structure of water.

**(6 Hours)**

### Unit – 4: Solid State

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

**(16 Hours)**

### Unit – 5: Ionic Equilibria

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

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

Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants.

Theory of acid–base indicators; selection of indicators and their limitations.

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).

**(20 Hours)**

### Reference Books:

- Atkins, P. W. & Paula, J. de Atkin's: *Physical Chemistry* 10<sup>th</sup> Ed., Oxford University Press (2006).
- Ball, D. W.: *Physical Chemistry*, Thomson Press, India (2007).
- Castellan, G. W.: *Physical Chemistry* 4<sup>th</sup> Ed. Narosa (2004).
- Mortimer, R. G. *Physical Chemistry* 3<sup>rd</sup> Ed. Elsevier: NOIDA, U.P. (2009).
- Puri, B. R., Sharma L. R., and Pathania M. S.: *Principle of Physical Chemistry*, Eds. 44<sup>th</sup>, Vishal Publishing Co., Jalandhar, (2010).

- Kotz J. C., Treichel P. M. & Townsend J. R.: *General Chemistry*, Cengage Learning India Pvt. Ltd., New Delhi (2009).
  - Crow, D. R.: *Principles and Applications of Electrochemistry*, Eds. 4<sup>th</sup>, Blackie Academic & Professional, Madras, (1994).
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## CHM P 112: Physical Chemistry – I Lab

(60 Hours)

### 1. Surface tension measurements.

- Determine the surface tension by (i) drop number (ii) drop weight method.
- Study the variation of surface tension of detergent solutions with concentration.
- Viscosity composition curve for a binary liquid mixture.

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

- Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.
- Study the variation of viscosity of sucrose solution with the concentration of solute.
- Surface tension composition curve for a binary liquid mixture.

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

### 4. pH metry

- Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
- Preparation of buffer solutions of different pH
  - Sodium acetate-acetic acid
  - Ammonium chloride-ammonium hydroxide
- pH metric titration of (i) strong acid *versus* strong base, (ii) weak acid *versus* strong base.
- Determination of dissociation constant of a weak acid.
- To study the dissociation constant of amino acid (glycine) and hence the isoelectric point of the acid.

*Any other experiment carried out in the class if permit.*

### 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* 8<sup>th</sup> Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry* 3<sup>rd</sup> Ed.; W.H. Freeman & Co.: New York (2003).
- Elias A. J., *A collection of Interesting General Chemistry Experiments*, University Press, India.

## SEMESTER – II

### CHM T 121: Organic Chemistry-I: Basics and Hydrocarbons

(Credits: Theory-04, Practicals-02)

Theory: 60 Hours

#### Unit – 1: Basics of Organic Chemistry

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

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

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

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

(6 Hours)

#### Unit -2: Stereochemistry

Fischer Projection, Newmann and Sawhorse Projection formulae and their interconversions; Geometrical isomerism: cis–trans and, syn-anti isomerism E/Z notations with C.I.P rules.

*Optical Isomerism:* Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers, Molecules with two or more chiral-centres, Distereoisomers, meso structures, Racemic mixture and resolution. Relative and absolute configuration: D/L and R/S designations.

(14 Hours)

#### Unit – 3: Chemistry of Aliphatic Hydrocarbons

##### A. Carbon-Carbon sigma bonds

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

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

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

*Reactions of alkenes:* Electrophilic additions their mechanisms (Markownikoff/ Anti Markownikoff addition), mechanism of oxymercuration-demercuration, 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**

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

**(20 Hours)**

### **Unit – 4: 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 Hours)**

### **Unit – 5: Polynuclear Hydrocarbons**

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

**(8 Hours)**

### **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.

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### **CHM P 121: Organic Chemistry – I Lab**

**(60 Hours)**

1. Checking the calibration of the thermometer
2. Purification of organic compounds by crystallization using the following solvents:
  - a. Water
  - b. Alcohol
  - c. Alcohol-Water
3. Determination of the melting points of above compounds and unknown organic

compounds (Kjeldahl method and electrically heated melting point apparatus)

4. Effect of impurities on the melting point – mixed melting point of two unknown organic compounds

5. Determination of boiling point of liquid compounds. (boiling point lower than and more than 100 °C by distillation and capillary method)

6. Chromatography

- a. Separation of a mixture of two amino acids by ascending and horizontal paper chromatography
- b. Separation of a mixture of two sugars by ascending paper chromatography
- c. Separation of a mixture of o-and p-nitrophenol or o-and p-aminophenol by thin layer chromatography (TLC)

### 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*, 5<sup>th</sup> Ed., Pearson (2012)

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## CHM T 122: Physical Chemistry – II: Chemical Thermodynamics and Chemical Equilibrium

(Credits: Theory-04, Practicals-02)  
Theory: 60 Hours

### Unit – 1: Chemical Thermodynamics – I

Introduction of different terms and processes in thermodynamics: [systems (isolated, closed, open) and surrounding, macroscopic properties (extensive and intensive), kinds of processes], state and path functions and their differentials. Zeroth law of thermodynamics.

*First Law*: concept of heat,  $q$ , work,  $w$ , internal energy,  $U$ , sign convention for heat and work; statement of first law; enthalpy,  $H$ ; heat capacities ( $C_v$ ,  $C_p$ ) and relation between them for ideal gases. Reversible and irreversible processes, maximum work; calculations of  $q$ ,  $w$ ,  $U$  and  $H$  for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions. Ideal gas law for adiabatic reversible expansion, comparison of adiabatic and isothermal reversible expansion. Joule-Thomson effect, Joule-Thomson coefficient in ideal and real (van der Waals) gases, inversion temperature.

(10 Hours)

### Unit – 2: Thermochemistry

Standard state, standard enthalpy of formation, Hess's Laws of constant heat summation and its application. Change in internal energy ( $\Delta U$ ) and enthalpy ( $\Delta H$ ) of chemical reactions, relation between  $\Delta U$  and  $\Delta H$ , variation of heat of reaction with temperature (Kirchhoff's equation). Enthalpy of neutralization. Bond Energy – Bond dissociation energy and its

calculation from thermo-chemical data. Adiabatic flame temperature and explosion temperature.

(8 Hours)

### Unit – 3: Chemical Thermodynamics – II

*Second Law:* Limitation of first Law, spontaneous processes and different statement of second law of thermodynamics, Carnot cycle and its efficiency, Carnot theorem; thermodynamic scale of temperature.

*Concept of Entropy:* Entropy changes in reversible and irreversible processes and of universe, physical concept of entropy (molecular and statistical interpretation of entropy), Calusius inequality; entropy as a function of  $V$  &  $T$ , and  $P$  &  $T$ ; entropy changes of an ideal gas in different processes, entropy change in mixing of gases.

*Free Energy Functions:* Free energy and its concept, Gibbs ( $G$ ) and Helmholtz ( $A$ ) free energies as thermodynamic quantities and their relationship; variation of free energy with temperature and pressure. Maxwell's relations, thermodynamic equation of state; criteria for reversible and irreversible processes (spontaneity); Gibbs-Helmholtz equations, its application of the determination of  $\Delta G$ ,  $\Delta H$ ,  $\Delta S$  of a reversible cell reaction.

*Third Law:* Variation of entropy with temperature (Nernst heat theorem), statement of third law, the concept of residual entropy. Applications of third law for determination of absolute entropies of liquid and gases.

(18 Hours)

### Unit – 4: Thermodynamic of Open System (Systems of Variable Composition)

Partial molal quantities, dependence of thermodynamic parameters on composition; the Gibbs-Duhem equation, chemical potential, variation of chemical potential with temperature and pressure, chemical potential in case of a system of ideal gases, chemical potential of real gases; concept and physical significance of fugacity, activity and activity coefficient, reference and standard states, thermodynamic functions of mixing ( $\Delta G_{\text{mix}}$ ,  $\Delta S_{\text{mix}}$ ,  $\Delta V_{\text{mix}}$ , and  $\Delta H_{\text{mix}}$ ) of ideal gases.

(10 Hours)

### Unit – 5: 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. Coupling of exoergic and endoergic reactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration; thermodynamic derivation of relations between the various equilibrium constants  $K_p$ ,  $K_c$  and  $K_x$ . Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

(14 Hours)

### Reference Books:

- Samuel Glasstone, *Thermodynamics for Chemistry*, Affiliated East-West Press, NewDelhi (2003).
- Atkins, P. W. & Paula, J. de Atkin's: *Physical Chemistry* 10<sup>th</sup> Ed., Oxford University Press (2006).
- Castellan, G. W. *Physical Chemistry* 4<sup>th</sup> Ed., Narosa (2004).

- Engel, T. & Reid, P. *Physical Chemistry 3<sup>rd</sup> Ed.*, Prentice-Hall (2012).
- McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: New Delhi (2004).
- Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. *Commonly Asked Questions in Thermodynamics*. CRC Press: NY (2011).
- Metz, C.R. *2000 Solved problems in chemistry*, Schaum Series (2006).

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## CHM P 122: Physical Chemistry – II Lab

(60 Hours)

### Thermochemistry:

- Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).
- Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
- Calculation of the enthalpy of ionization of ethanoic acid.
- Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.
- Determination of basicity/proticity of a poly-protic acid by the thermo-chemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.
- Determination of enthalpy of hydration of copper sulphate.
- Study of the solubility of benzoic acid in water and determination of  $\Delta H$ .

### Chemical Equilibrium:

- Equilibrium constant of methyl acetate hydrolysis reaction.

*Any other experiment carried out in the class if permit.*

### 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).

## SEMESTER – III

### CHM T 211: Inorganic Chemistry – II: Radioactivity & Chemistry of s-and p-Block elements

(Credits: Theory-04, Practicals-02)

Theory: 60 Hours

#### Unit – 1: Radioactivity

Radioactive decay, half life and average life of radio elements, units of radioactivity, natural radioactive disintegration series, Instrumental analysis of radioactive elements, radioactive equilibrium, group displacement law, isotope, isotone, isobars and nuclear isomerism. Application of isotope in medicine, agriculture, reaction mechanism (isotope as tracer), age of minerals, age of earth, radio carbon dating, nuclear particles, nuclear forces: meson exchange theory.

Nuclear models (elementary idea), nuclear stability, nuclear binding energy, nuclear reactions, magic numbers, mass defect, proton-neutron ratio, packing fraction, Artificial radioactivity, transmutation of elements, fission, fusion and spallation reaction. Nuclear energy, hazards of nuclear radiations and safety measures.

(14 Hours)

#### Unit – 2: Acid and Bases

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

(8 Hours)

#### Unit – 3: Chemistry of *s* and *p* Block Elements

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

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

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

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

(20 Hours)

#### Unit – 4: Noble Gases

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of XeF<sub>2</sub>, XeF<sub>4</sub> and XeF<sub>6</sub>; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF<sub>2</sub>). Molecular shapes of noble gas compounds (VSEPR theory).

(10 Hours)

#### Unit – 5: Inorganic Polymers

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

(8 Hours)

**Reference Books:**

- Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
- 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.
- Greenwood, N.N. & Earnshaw. *Chemistry of the Elements*, Butterworth-Heinemann. 1997.
- Cotton, F.A. & Wilkinson, G. *Advanced Inorganic Chemistry*, Wiley, VCH, 1999.
- Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry 4<sup>th</sup> Ed.*, Pearson, 2010.
- Shriver & Atkins, *Inorganic Chemistry 5<sup>th</sup> Ed.*

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**CHM P 211: Inorganic Chemistry – II Lab**

(60 Hours)

**(A) Iodo / Iodimetric Titrations**

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

**(B) Gravimetric Analysis:**

- Estimation of nickel (II) using Dimethylglyoxime (DMG).
- Estimation of copper as  $CuSCN$
- Estimation of iron as  $Fe_2O_3$  by precipitating iron as  $Fe(OH)_3$ .
- Estimation of Al (III) by precipitating with oxine and weighing as  $Al(oxine)_3$  (aluminium oxinate).

**(C) Inorganic preparations**

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

**Reference Books:**

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

**CHM T 212: Organic Chemistry-II: Oxygen Containing Functional Groups**

(Credits: Theory-04, Practicals-02)

Theory: 60 Hours

**Unit – 1: Chemistry of Halogenated Hydrocarbons**

*Alkyl halides:* Methods of preparation, nucleophilic substitution reactions –  $S_N^1$ ,  $S_N^2$  and  $S_N^i$  mechanisms with stereochemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination.

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

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

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

**(16 Hours)**

## **Unit – 2: Alcohols, Phenols, Ethers and Epoxides**

*Alcohols:* preparation, properties and relative reactivity of  $1^\circ$ ,  $2^\circ$ ,  $3^\circ$  alcohols, Bouvaelt-Blanc Reduction; Preparation and properties of glycols: Oxidation by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement:

*Phenols:* Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer–Tiemann and Kolbe’s–Schmidt Reactions, Fries and Claisen rearrangements with mechanism;

*Ethers and Epoxides:* Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and  $LiAlH_4$

**(16 Hours)**

## **Unit – 3: Carbonyl Compounds**

Structure, reactivity and preparation

Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisan-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation,  $\alpha$ -substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner,  $LiAlH_4$ ,  $NaBH_4$ , MPV, PDC and PGC)

Addition reactions of unsaturated carbonyl compounds: Michael addition.

Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

**(14 Hours)**

## **Unit – 4: Carboxylic Acids and their Derivatives**

Preparation, physical properties and reactions of monocarboxylic acids: Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids

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

(10 Hours)

## Unit – 5: Sulphur containing compounds

Preparation and reactions of thiols, thioethers and sulphonic acids.

(4 Hours)

### Reference Books:

- Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. *Organic Chemistry (Volume I)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc.

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## CHM P 212: Organic Chemistry – II Lab

(60 Hours)

1. Functional group tests for alcohols, phenols, carbonyl and carboxylic acid group.
2. Organic preparations:
  - i. Acetylation of one of the following compounds: amines (aniline, *o*-, *m*-, *p*-toluidines and *o*-, *m*-, *p*-anisidine) and phenols ( $\beta$ -naphthol, vanillin, salicylic acid) by any one method:
    - a. Using conventional method.
    - b. Using green approach
  - ii. Benzoylation of one of the following amines (aniline, *o*-, *m*-, *p*-toluidines and *o*-, *m*-, *p*-anisidine) and one of the following phenols ( $\beta$ -naphthol, resorcinol, *p*-cresol) by Schotten-Baumann reaction.
  - iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).
  - iv. Bromination of any one of the following:
    - a. Acetanilide by conventional methods
    - b. Acetanilide using green approach (Bromate-bromide method)
  - v. Nitration of any one of the following:
    - a. Acetanilide/nitrobenzene by conventional method
    - b. Salicylic acid by green approach (using ceric ammonium nitrate).
  - vi. Selective reduction of *meta* dinitrobenzene to *m*-nitroaniline.
  - vii. Reduction of *p*-nitrobenzaldehyde by sodium borohydride.
  - viii. Hydrolysis of amides and esters.
  - ix. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.
  - x. *S*-Benzylisothiuronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
  - xi. Aldol condensation using either conventional or green method.
  - xii. Benzil-Benzilic acid rearrangement.
  - xiii. Beckman Rearrangement

The above derivatives should be prepared using 0.5-1g of the organic compound.

The solid samples must be collected and may be used for recrystallization, melting point and TLC.

## 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*, 5<sup>th</sup> 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 (2002).

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## CHM P 213: Physical Chemistry-III: Phase Equilibria, Solution and Chemical Kinetics (Credits: Theory-04, Practicals-02) Theory: 60 Hours

### Unit – 1: Phase Equilibrium

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Phase diagrams with applications for one-component systems (water and sulfur) and two component systems involving eutectics, congruent, incongruent melting points and solid solution (lead-silver,  $\text{FeCl}_3\text{-H}_2\text{O}$  and Na-K *etc.*).

Three Component System: Graphical representation of three component system; system of three liquids: having partial miscibility.

**Type-I**            Formation of one pair of partially miscible liquids

**Type-II**           Formation of two pairs of partially miscible liquids

**Type-III**          Formation of three pairs of partially miscible liquids

(15 Hours)

### Unit – 2: Phase Transformation

Stability of phases; Clapeyron equation; Clausius-Clapeyron equation and its applications to solid- liquid, liquid-vapor and solid-vapor equilibria. Thermodynamics of phase transition; classification of phases - bubbles, cavities and droplets-Kelvin equation.

(8 Hours)

### Unit – 3: Solutions and Colligative Properties

The chemical potential of liquids; ideal solutions; lowering of vapor pressure, Raoult's and Henry's Laws and their applications. Excess thermodynamic functions.

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

Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and non-ideal), vapor pressure-composition and temperature-composition curves of ideal and non-ideal solution; distillation of solution, Lever rule, azeotropes. Partial miscibility of liquids, CST, miscible pairs, Immiscibility of liquids – Principle of steam distillation.

Nernst distribution law: its derivation and applications.

**(19 Hours)**

#### **Unit – 4: Chemical Kinetics**

The concept of reaction rate, 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; half life of a reaction.

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

**(10 Hours)**

#### **Unit – 5: Complex Reactions**

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 (v) uni molecular gas reaction (Lindemann mechanism)

**(8 Hours)**

#### **Reference Books:**

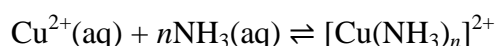
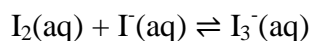
- Peter, A. & Paula, J. de. *Physical Chemistry* 9<sup>th</sup> Ed., Oxford University Press (2011).
- Castellan, G. W. *Physical Chemistry* 4<sup>th</sup> Ed., Narosa (2004).
- Engel, T. & Reid, P. *Physical Chemistry* 3<sup>rd</sup> Ed., Prentice-Hall (2012).
- Laidler, K. J.; *Chemical Kinetics*, Eds: 3<sup>rd</sup>, Pearson, New Delhi, 2011.
- Rajaram, J. and Kuriacose, J. C.; *Kinetics and Mechanisms of Chemical Transformations Applications of Femto-chemistry*, MacMillan, New Delhi, 2011.
- McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: New Delhi (2004).
- Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. *Commonly Asked Questions in Thermodynamics*. CRC Press: NY (2011).
- Levine, I. N. *Physical Chemistry* 6<sup>th</sup> Ed., Tata Mc Graw Hill (2010).
- Metz, C.R. *2000 solved problems in chemistry*, Schaum Series (2006).
- Zundhal, S.S. *Chemistry concepts and applications* Cengage India (2011).

#### **CHM P 213: Physical Chemistry – III Lab**

**(60 Hours)**

1. Determination of critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.

2. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method:
  - a. simple eutectic and
  - b. congruently melting systems
3. Distribution of acetic/ benzoic acid between water and cyclohexane.
4. Study the equilibrium of at least one of the following reactions by the distribution method:



5. Study the kinetics of the following reactions.
  - a. Initial rate method: Iodide-persulphate reaction.
  - b. Order of reaction of  $\text{I}_2$  – acetone –  $\text{H}^+$  ion.
  - c. Integrated rate method:
    - (i) Acid hydrolysis of methyl acetate with hydrochloric acid
    - (ii) Saponification of ethyl acetate.
  - d. Compare the strengths of  $\text{HCl}$  and  $\text{H}_2\text{SO}_4$  by studying kinetics of hydrolysis of methyl acetate.

#### 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* 8<sup>th</sup> Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry* 3<sup>rd</sup> Ed.; W.H. Freeman & Co.: New York (2003).
- Rose, J.: *Advanced Physico-Chemical Experiments*, Sir Isaac Pitman & Sons Ltd, London.

## SEMESTER – IV

### CHM T 221: Inorganic Chemistry – III: Coordination Chemistry

(Credits: Theory-04, Practicals-02)

Theory: 60 Hours

#### Unit – 1: Coordination Chemistry

Werner's theory, IUPAC nomenclature of coordination compounds, Types of isomerism in coordination compounds: Constitutional, geometrical and optical isomerism in respect of coordination numbers 4 and 6, Determination of configuration of cis-, trans-isomers by chemical methods.

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

(20 Hours)

#### Unit – 2: Electronic Spectra of Transition Metal Complex

Introduction to electronic spectra of transition metal complexes, Orgel diagrams for  $3d^1$ - $3d^9$  ions, selection rules, d-d/charge transfer spectra, Colour, spectrochemical series, Nephelauxetic effect, trans effect, (example and applications) labile and inert complexes. Difference between the first, second and third transition series.

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

(10 Hours)

#### Unit – 3: Magnetic Properties of Transition Metal Complex

Types of magnetic behaviour, methods of determining magnetic susceptibility, spin only formula, L-S coupling, Orbital contribution to magnetic moments, quenching of magnetic moment, super-exchange, antiferromagnetic interaction (elementary idea with examples only), application of spin only values of magnetic moments to determine valency and stereochemistry of coordination compounds (based on VBT and CFT).

(10 Hours)

#### Unit – 4: Chemistry of Lanthanoids and Actinoids

Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides and actinides (ion-exchange method only), important lanthanide compounds, similarities the later actinides and lanthanides elements.

(6 Hours)

#### Unit – 5: Bioinorganic Chemistry

Elements of life: essential major, trace and ultratrace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially  $Na^+$ ,  $K^+$ ,  $Mg^{+2}$ ,  $Ca^{+2}$ ,  $Fe^{3+/2+}$ ,  $Cu^{+2}$ , and  $Zn^{+2}$ ). Haemoglobin, myoglobin, chlorophyll, cytochromes, ferredoxins and carbonic anhydrase-their structural features and functions in living system.

Toxic metal ions and their effects, lead, mercury, cadmium and arsenic poisoning, organo-mercury compounds; Use of chelating agents in medicine: Wilson diseases, detoxification of metal ions – chelation therapy (simple idea with some examples of chelating drugs). Pt and Au complexes as drugs (examples only), metal dependent diseases.

(14 Hours)

**Reference Books:**

- Purcell, K.F & Kotz, J.C. Inorganic Chemistry W.B. Saunders Co, 1977.
  - Huheey, J.E., Inorganic Chemistry, Prentice Hall, 1993.
  - Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994.
  - 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.
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**CHM P 221: Inorganic Chemistry – III Lab**

(60 Hours)

**(A) Inorganic Preparations:**

- i. Tetraamminecopper (II) sulphate,  $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$
- ii. *Cis* and *trans*  $\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2 \cdot (\text{H}_2\text{O})_2]$  Potassium dioxalatodiaquachromate (III)
- iii. Tetraamminecarbonatocobalt (III) ion
- iv. Potassium tris(oxalate)ferrate(III)

**(B) Quantitative Estimation of Metal Ions in Binary Mixture**

- i. Estimation of Iron (II/III) and Calcium (II) in a Mixture
- ii. Estimation of Fe(III) and Mn (II) in a Mixture
- iii. Estimation of Fe(III) and Cu(II) in a Mixture
- iv. Estimation of Fe(III) and Zn(II) in a Mixture

**(C) Chromatography of metal ions**

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

- i. Ni (II) and Co (II)
- ii. Fe (III) and Al (III)

**Reference Book:**

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

## CHM T 222: Organic Chemistry-III: Introduction of N – Containing Functional Group Towards Heterocyclic Chemistry

(Credits: Theory-04, Practicals-02)  
Theory: 60 Hours

### Unit – 1: Nitrogen Containing Functional Groups

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

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

Diazonium Salts: Preparation and their synthetic applications.

(18 Hours)

### Unit – 2: Heterocyclic Compounds

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

Derivatives of furan: Furfural and furoic acid.

(22 Hours)

### Unit – 3: Alkaloids

Natural occurrence, General structural features, Isolation and their physiological action

Hoffmann's exhaustive methylation, Emde's modification, Structure elucidation and synthesis of Hygrine and Nicotine. Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine, and Reserpine.

(10 Hours)

### Unit – 4: Terpenes

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

(10 Hours)

### Reference 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 1<sup>st</sup> 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*, Prajati Parakashan (2010)

### CHM P 222: Organic Chemistry – III Lab

(60 Hours)

1. Detection of extra elements.
2. Functional group test for nitro, amine and amide groups.
3. Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols and carbonyl compounds)

### 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, 5<sup>th</sup> 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).

### CHM T 223: Physical Chemistry-IV: Catalysis, Electro & Photo-Chemistry

(Credits: Theory-04, Practicals-02)

Theory: 60 Hours

#### Unit – 1: Catalysis

Type of catalysts, specificity and selectivity, mechanism of catalyzed reaction at solid surface; effect of temperature on surface reaction, promoters and poisons, effect of particle size and efficiency of nanoparticles as catalysts; enzyme catalysis, Michaelis-Menten mechanism, effect of temperature and pH on enzyme catalysis; acid-base catalysis.

(10 Hours)

#### Unit – 2: Surface and Colloidal Chemistry

Physical adsorption, chemisorptions, nature of adsorbed state, adsorption isotherm; Langmuir and Freundlich adsorption isotherms. Multi layer adsorption-BET equation (no derivation) and its application to surface area measurement.

Colloidal state; definition of colloids, classification of colloids. Solids in liquids (sols); properties– kinetic, optical and electrical, stability of colloids, protective action; Hardy-Schulze law, gold number. Liquids in liquids (Emulsions): types of emulsions (micelles and reverse micelles), preparation, emulsifier. Liquid in solid (gels): classification, preparation, and properties, general application of colloids.

**(10 Hours)**

### **Unit – 3: Conductance**

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

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

**(15 Hours)**

### **Unit – 4: Electrochemistry**

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

Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Single electrode potential, its measurement and sign convention. Standard electrode (reduction) potential, and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and  $\text{SbO/Sb}_2\text{O}_3$  electrodes (iv) qualitative discussion of potentiometric titrations (acid-base, redox, precipitation). Concentration cells with and without transference, liquid junction potential and its elimination; determination of activity coefficients and transference numbers. Fuel cell (Hydrogen-Oxygen), Commercial Cell (Primary & Secondary cell), dry cell, acid-alkali storage cell & introduction of lithium ion cells.

**(15 Hours)**

### **Unit – 4: Photochemistry**

Characteristics of electromagnetic radiation and interaction of radiation with matter, difference between thermal and photochemical processes. Laws of photochemistry: Grothus-Draper law, Stark-Einstein law, Jablonski diagram depicting various processes occurring in the excited state, qualitative description of fluorescence, phosphorescence, non-radiative processes (internal conversion, intersystem crossing). Lambert-Beer's law and its limitation,

physical significance of absorption coefficient; quantum efficiency, reasons for low and high quantum efficiency. Kinetics of photochemical reactions ( $\text{H}_2 + \text{Br}_2 = \text{HBr}$  and  $2\text{HI} = \text{H}_2 + \text{I}_2$ ), photostationary state. Chemical actinometers (ferri-oxalate, uranyl oxalate, MGL [malachite green leucocyanide]) and Reinecke's salt); chemiluminescence, role of photochemical reactions in biological process.

(10 Hours)

#### Reference Books:

- Peter, A. & Paula, J. de. *Physical Chemistry* 9<sup>th</sup> Ed., Oxford University Press (2011).
- Castellan, G. W. *Physical Chemistry* 4<sup>th</sup> Ed., Narosa (2004).
- Engel, T. & Reid, P. *Physical Chemistry* 3<sup>rd</sup> Ed., Prentice-Hall (2012).
- Barrow, G. M., *Physical Chemistry* 5<sup>th</sup> Ed., Tata McGraw Hill: New Delhi (2006).
- Mortimer, R. G. *Physical Chemistry* 3<sup>rd</sup> Ed., Elsevier: NOIDA, UP (2009).
- Rogers, D. W. *Concise Physical Chemistry* Wiley (2010).
- Silbey, R. J.; Alberty, R. A. & Bawendi, M. G. *Physical Chemistry* 4<sup>th</sup> Ed., John Wiley & Sons, Inc. (2005).
- Laidler, K. J.; *Chemical Kinetics*, Eds: 3<sup>rd</sup>, Pearson, New Delhi, 2011.
- Crow, D. R: *Principles and Applications of Electrochemistry*, Eds. 4<sup>th</sup>, Blackie Academic & Professional, Madras, 1994.

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#### CHM P 223: Physical Chemistry – IV Lab

(60 Hours)

##### Catalysis:

1. Kinetics of enzymation reaction (starch-amylase system).
2. Kinetics of catalytic decomposition of  $\text{H}_2\text{O}_2$

##### Surface Chemistry:

- Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

##### Conductometry:

- Determination of cell constant.
- Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
- Perform the following conductometric titrations:
  - (i) Strong acid *versus* strong base
  - (ii) Weak acid *versus* strong base
  - (iii) Dibasic acid *versus* strong base
  - (iv) Potassium dichromate *versus* Mohr's salt

##### Potentiometry:

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

### **Photochemistry:**

- Photochemical reduction of ferric oxalate in cyanotype blue printing.

### **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* 8<sup>th</sup> Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry* 3<sup>rd</sup> Ed.; W.H. Freeman & Co.: New York (2003).
- Elias A. J., *A collection of Interesting General Chemistry Experiments*, University Press, India.
- Rose, J.: *Advanced Physico-Chemical Experiments*, Sir Isaac Pitman & Sons Ltd, London.

## SEMESTER – V

### CHM T 311: Organic Chemistry – IV: Biomolecules

(Credits: Theory-04, Practical-02)  
Theory: 60 Hours

#### Unit – 1: Nucleic Acids

Components of nucleic acids, Nucleosides and nucleotides

Structure, synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine  
Structure of polynucleotides.

(9 Hours)

#### Unit – 2: Amino Acids, Peptides and Proteins

Amino acids, Peptides and their classification.

$\alpha$ -Amino Acids - Synthesis, ionic properties and reactions. Zwitterions,  $pK_a$  values, isoelectric point and electrophoresis

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

(16 Hours)

#### Unit – 3: Enzymes

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

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

(8 Hours)

#### Unit – 4: 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.

(8 Hours)

#### Unit – 5: Concept of Energy in Biosystems

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

Introduction to metabolism (catabolism, anabolism).

ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change. Agents for transfer of electrons in biological redox systems:  $NAD^+$ , FAD.

Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle.

Overview of catabolic pathways of fat and protein.

Interrelationship in the metabolic pathways of protein, fat and carbohydrate. Caloric value of food, standard caloric content of food types.

**(7 Hours)**

#### **Unit – 6: Pharmaceutical Compounds: Structure and Importance**

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis). An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

**(12 Hours)**

#### **Reference 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.

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#### **CHM P 311: Organic Chemistry – IV Lab**

**(60 Hours)**

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.

#### **Reference Books:**

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

#### **CHM T 312: Physical Chemistry – V: Quantum Chemistry and Spectroscopy**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Hours**

#### **Unit – 1: Quantum Chemistry – I**

A review of quantum mechanics versus classical mechanics, (black body radiation, photoelectric effect, Compton's effect), wave nature of electron; wave particle duality; Heisenberg's uncertainty principle.

Schrödinger wave equation: wave function and interpretation, wave functions and probabilities; normalization and orthogonality of wave functions; time-independent Schrödinger equations.

Operators and their algebra, linear and Hermitian operators, quantum mechanical operators for the dynamic variables; eigenfunctions, eigenvalues and eigen value equation, average value and the expectation value of the physical quantities; expansion of arbitrary state in term of complete set; postulates of quantum mechanics.

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

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

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

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

**(12 Hours)**

## **Unit – 2: Quantum Chemistry – II**

Qualitative treatment of hydrogen and hydrogen like atoms, setting up of Schrödinger wave equation in spherical polar coordinate; separation into three equation of variables, R, theta and phi (without derivation), introduction of the four quantum numbers and their interdependence on the basis of the solutions of the three equations, total wave function, expression for the energy, probability density function, radial and angular plots., expressions for the total wave function for 1s, 2s, 2p and 3d orbitals of hydrogen.

Application of the Schrödinger equation to two or more (many) electron systems, limitations of the equation, need for the approximate solutions, methods of obtaining the approximate solution of the Schrödinger wave equation. The variation principle (particle-in-a-box, harmonic oscillator, hydrogen atom), electron spin, Pauli antisymmetry principle; application to the two electron system for ground and excited state He atom.

**(12 Hours)**

## **Unit – 3: Molecular Spectroscopy – I**

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

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

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

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

(12 Hours)

#### Unit – 4: Molecular Spectroscopy – II

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

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

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

(12 Hours)

#### UNIT – 5: Electrical & Magnetic Properties of Atoms and Molecules

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

(12 Hours)

#### Reference Books:

- Atkins, P. and Friedman, R.; *Molecular Quantum Mechanics*, Eds: 5<sup>th</sup>, Oxford University Press, 2011.
- Chandra, A. K.: *Introductory Quantum Chemistry*, Eds: 4<sup>th</sup>, Tata McGraw Hill, New Delhi, 1994.
- Levine, I. N.: *Quantum Chemistry*, Eds: 5<sup>th</sup>, PHI, 2000.
- Engel, T. and Reid, P.: *Quantum Chemistry and Spectroscopy*, Pearson, 2011, New Delhi.
- Prasad, R. K.: *Quantum Chemistry*, Eds: 4<sup>th</sup>, New Age Inter. Pub., 2010.
- Banwell, C. N. and McCash, E. M.: *Fundamentals of Molecular Spectroscopy*, Ed. 4<sup>th</sup>, Tata McGraw-Hill, 1994.
- G. M. Barrow: *Introduction to Molecular Spectroscopy*
- Kakkar, R. Atomic & Molecular Spectroscopy, Cambridge University Press (2015)

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**CHM P 312: Physical Chemistry – V Lab**  
**Hours)**

**(60**

### UV/Visible spectroscopy:

- Study the 200-500 nm absorbance spectra of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  (in 0.1 M  $\text{H}_2\text{SO}_4$ ) and determine the  $\lambda_{\text{max}}$  values. Calculate the energies of the two transitions in different units ( $\text{J molecule}^{-1}$ ,  $\text{kJ mol}^{-1}$ ,  $\text{cm}^{-1}$ , eV).
- Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of  $\text{K}_2\text{Cr}_2\text{O}_7$ .
- Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

### Colorimetry:

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

### Reference Books:

- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry* 8<sup>th</sup> Ed.; McGraw-Hill: New York (2003).
- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry* 3<sup>rd</sup> Ed.; W.H. Freeman & Co.: New York (2003).
- Elias A. J.: *A collection of Interesting General Chemistry Experiments*, University Press, India.
- Yadav J. B.: *Advanced Practical Physical Chemistry*, Krishna Prakashan Media (P) Ltd. Meerut.

## SEMSETER – VI

### CHM T 321: Inorganic Chemistry-IV: Organometallic Chemistry

(Credits: Theory-04, Practicals-02)

Theory: 60 Hours

#### Unit – 1: Theoretical Principles in Qualitative Analysis (H<sub>2</sub>S Scheme)

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

(10 Hours)

#### Unit – 2: 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. Role of triethylaluminium in polymerisation of ethene (Ziegler – Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium.

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

(22 Hours)

#### Unit – 3: Reaction Kinetics and Mechanism

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

(10 Hours)

#### Unit – 4: Catalysis by Organometallic Compounds

Study of the following industrial processes and their mechanism:

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

(10 Hours)

### Unit – 5: Complexometric Titration

Complexones, masking and demasking interactions, metallochrome indicators, titration of metal ions and their mixtures with EDTA, hardness of water and its determination

(8 Hours)

#### Reference Books:

- Vogel, A.I. *Qualitative Inorganic Analysis*, Longman, 1972
- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall, 1996-03-07.
- Cotton, F.A. G.; Wilkinson & Gaus, P.L. *Basic Inorganic Chemistry 3<sup>rd</sup> Ed.*; Wiley India,
- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity 4<sup>th</sup> Ed.*, Harper Collins 1993, Pearson, 2006.
- Sharpe, A.G. *Inorganic Chemistry*, 4<sup>th</sup> Indian Reprint (Pearson Education) 2005
- Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry 3<sup>rd</sup> Ed.*, John Wiley and Sons, NY, 1994.
- Greenwood, N.N. & Earnshaw, A. *Chemistry of the Elements, Elsevier 2<sup>nd</sup> Ed*, 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. & P. Atkins, *Inorganic Chemistry 2<sup>nd</sup> Ed.*, Oxford University Press, 1994.
- Basolo, F. & Person, R. *Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution 2<sup>nd</sup> Ed.*, John Wiley & Sons Inc; NY.
- Purcell, K.F. & Kotz, J.C., *Inorganic Chemistry*, W.B. Saunders Co. 1977
- Miessler, G. L. & Donald, A. Tarr, *Inorganic Chemistry 4<sup>th</sup> Ed.*, Pearson, 2010.
- Collman, James P. et al. *Principles and Applications of Organotransition Metal Chemistry*. Mill Valley, CA: University Science Books, 1987.
- Crabtree, Robert H. *The Organometallic Chemistry of the Transition Metals. j* New York, NY: John Wiley, 2000.
- Spessard, Gary O., & Gary L. Miessler. *Organometallic Chemistry*. Upper Saddle River, NJ: Prentice-Hall, 1996.

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### CHM P 321: Inorganic Chemistry – IV Lab

(60 Hours)

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:

$\text{CO}_3^{2-}$ ,  $\text{NO}_2^-$ ,  $\text{S}^{2-}$ ,  $\text{SO}_3^{2-}$ ,  $\text{S}_2\text{O}_3^{2-}$ ,  $\text{CH}_3\text{COO}^-$ ,  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{NO}_3^-$ ,  $\text{BO}_3^{3-}$ ,  $\text{C}_2\text{O}_4^{2-}$ ,  $\text{PO}_4^{3-}$ ,  $\text{NH}_4^+$ ,  $\text{K}^+$ ,  $\text{Pb}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Bi}^{3+}$ ,  $\text{Sn}^{2+}$ ,  $\text{Sb}^{3+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$

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<sub>3</sub><sup>2-</sup> and SO<sub>3</sub><sup>2-</sup>, NO<sub>2</sub><sup>-</sup> and NO<sub>3</sub><sup>-</sup>, Cl<sup>-</sup> and Br<sup>-</sup>, Cl<sup>-</sup> and I<sup>-</sup>, Br<sup>-</sup> and I<sup>-</sup>, NO<sub>3</sub><sup>-</sup> and Br<sup>-</sup>, NO<sub>3</sub><sup>-</sup> and I<sup>-</sup>.

Spot tests should be done whenever possible

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

### Reference Books

- Vogel's *Qualitative Inorganic Analysis*, Revised by G. Svehla.
- Marr & Rockett *Inorganic Preparations*.
- Ghosal, Mahapatra and Nad, *An Advanced Course in Practical Chemistry*.

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## CHM T 322: Organic Chemistry – V: Spectroscopy

(Credits: Theory-04, Practicals-02)  
Theory: 60 Hours

### Unit - 1: 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, Interpretation of NMR spectra of simple compounds.

Applications of IR, UV and NMR for identification of simple organic molecules.

(24 Hours)

## Unit - 2: 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 Hours)**

## Unit – 3: Dyes

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing, Synthesis and applications of: Azo dyes – Methyl Orange and Congo Red (mechanism of Diazo Coupling); Triphenyl Methane Dyes -Malachite Green, Rosaniline and Crystal Violet; Phthalein Dyes – Phenolphthalein and Fluorescein; Natural dyes –structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes with examples.

**(8 Hours)**

## Unit – 4: Polymers

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

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

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

**(12 Hours)**

## Reference Books:

- Kalsi, P. S. *Textbook of Organic Chemistry 1<sup>st</sup> 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.
  - Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry*, Oxford University Press.
  - Singh, J.; Ali, S.M. & Singh, J. *Natural Product Chemistry*, Prajati Prakashan (2010).
  - Kemp, W. *Organic Spectroscopy*, Palgrave
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### CHM P 322: Organic Chemistry – V Lab

(60 Hours)

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

### Reference 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*, 5<sup>th</sup> 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).

## **\*Discipline Specific Elective (DSE) in Chemistry**

### **CHM T 313-314 and 323-324**

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#### **DSE – A: Applications of Computers in Chemistry**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Hours**

##### **Unit – 1: Basics**

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

**(30 Hours)**

##### **Unit – 2: Numerical methods**

*Roots of equations:* Numerical methods for roots of equations: Quadratic formula, iterative method, Newton-Raphson method, Binary bisection and Regula-Falsi.

*Differential calculus:* Numerical differentiation.

*Integral calculus:* Numerical integration (Trapezoidal and Simpson's rule), probability distributions and mean values.

*Simultaneous equations:* Matrix manipulation: addition, multiplication. Gauss-Siedal method.

*Interpolation, extrapolation and curve fitting:* Handling of experimental data.

*Conceptual background of molecular modelling:* Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

**(30 Hours)**

##### **Reference Books:**

- Harris, D. C. *Quantitative Chemical Analysis*. 6<sup>th</sup> 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.
- Noggle, J. H. *Physical chemistry on a Microcomputer*. Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).

#### **DSE – A Lab: Applications of Computers in chemistry**

**(60 Hours)**

Computer programs based on numerical methods for

1. Roots of equations: (e.g. volume of van der Waals gas and comparison with ideal gas, pH of a weak acid).
2. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
3. Numerical integration (e.g. entropy/ enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values.
4. Matrix operations. Application of Gauss-Siedel method in colourimetry.
5. Simple exercises using molecular visualization software.

### Reference Books:

- McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
- Mortimer, R. *Mathematics for Physical Chemistry*. 3<sup>rd</sup> Ed. Elsevier (2005).
- Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
- Yates, P. *Chemical Calculations*. 2<sup>nd</sup> Ed. CRC Press (2007).
- Harris, D. C. *Quantitative Chemical Analysis*. 6<sup>th</sup> 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.
- Noggle, J. H. *Physical Chemistry on a Microcomputer*. Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).

## DSE – B: Analytical Methods in Chemistry

(Credits: Theory-04, Practicals-02)  
Theory: 60 Hours

### Unit – 1: Qualitative and quantitative aspects of analysis

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

(5 Hours)

### Unit – 2: 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. Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.

*Infrared Spectrometry:* Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.

Structural illustration through interpretation of data, Effect and importance of isotope substitution.

*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 Hours)**

### **Unit – 3: Thermal methods of analysis:**

Theory of thermogravimetry (TG), basic principle of instrumentation.

Techniques for quantitative estimation of Ca and Mg from their mixture.

**(5 Hours)**

### **Unit – 4: 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  $pK_a$  values.

**(10 Hours)**

### **Unit – 5: 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 nonaqueous media.

Chromatography: Classification, principle and efficiency of the technique.

Mechanism of separation: adsorption, partition & ion exchange.

Development of chromatograms: frontal, elution and displacement methods.

Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

Stereoisomeric separation and analysis: Measurement of optical rotation, calculation of Enantiomeric excess (ee)/ diastereomeric excess (de) ratios and determination of enantiomeric composition using NMR, Chiral solvents and chiral shift reagents. Chiral chromatographic techniques using chiral columns (GC and HPLC).

Role of computers in instrumental methods of analysis.

**(15 Hours)**

## Reference Books:

- Vogel, Arthur I: A Test 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, Hobert 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.
  - Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
  - Ditts, R.V. Analytical Chemistry – Methods of separation.
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## DSE – B Lab: Analytical Methods in Chemistry

(60 Hours)

### I. Separation Techniques

#### 1. Chromatography:

##### (a) Separation of mixtures

- (i) Paper chromatographic separation of  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$ , and  $\text{Cr}^{3+}$ .
- (ii) Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the  $R_f$  values.
- (b) Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their  $R_f$  values.
- (c) Chromatographic separation of the active ingredients of plants, flowers and juices by TLC

### II. Solvent Extractions:

- (i) To separate a mixture of  $\text{Ni}^{2+}$  &  $\text{Fe}^{2+}$  by complexation with DMG and extracting the  $\text{Ni}^{2+}$ -DMG complex in chloroform, and determine its concentration by spectrophotometry.
  - (ii) Solvent extraction: separation from a mixture of irons and gallium.
3. Determine the pH of the given aerated drinks fruit juices, shampoos and soaps.

4. Determination of Na, Ca, Li in cola drinks and fruit juices using flame photometric techniques.

5. Analysis of soil:

- (i) Determination of pH of soil.
- (ii) Total soluble salt
- (iii) Estimation of calcium, magnesium, phosphate, nitrate

#### **6. Quantitative Estimation of Metal Ions in Binary Mixture**

- (i) Estimation of Iron (II/III) and Calcium (II) in a Mixture
- (ii) Estimation of Fe(III) and Mn (II) in a Mixture
- (iii) Estimation of Fe(III) and Cu(II) in a Mixture
- (iv) Estimation of Fe(III) and Zn(II) in a Mixture

### **III Spectrophotometry**

- 1. Determination of  $pK_a$  values of indicator using spectrophotometry.
- 2. Structural characterization of compounds by infrared spectroscopy.
- 3. Determination of dissolved oxygen in water.
- 4. Determination of chemical oxygen demand (COD).
- 5. Determination of Biological oxygen demand (BOD).
- 6. Determine the composition of the Ferric-salicylate/ ferric-thiocyanate complex by Job's method.

#### **Reference 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, Hobert 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.
- Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
- Ditts, R.V. Analytical Chemistry – Methods of separation.

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#### **DSE – C: Basics of Drug Design & Medicinal Chemistry**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Hours**

#### **Unit – 1: Basic Concept of Drug Design & Physiochemical Factors**

Introduction; Basics of drug design; analog and Prodrug; Concept of lead; Factors governing drug design; Rational approach to drug design.

Physical-Chemical factors and biological activities; Factors governing ability of drug to reach active site.

(12 Hours)

## **Unit – 2: Molecular Modeling & Ligand Design Concept**

Concept of structure of drug molecules and its optimization; Molecular modeling and drug design; Basic concept of Protein and its structure; Structure based drug design; Ligand receptor recognition; Active site of a target molecules; Characterization of site and design of ligands.

(12 Hours)

## **Unit – 3: Analgesic & Antimalarial Drugs**

Concept of Analgesics drug; Synthesis and use of analgesics drugs: Paracetamol, Phenacetine, Acetanilide, Aspirin, Salol, Cinchophene, and Phenazone.

Antimalarial Drugs: Synthesis and use of Chloroquine phosphate.

(12 Hours)

## **Unit - 4: Antibacterial & Antibiotic**

Sulphonamide drugs: Antibacterial properties.

Synthesis and use of Sulphonamide drugs: Sulphanilide, Sulphapyridine, Sulphathiazole, Sulphadiazine,

Concept of Antibiotics with its application.

(12 Hours)

## **Unit – 5: Herbal medicine**

Herbal Drug: Its importance

Ethanobotanical survey methods; introduction to ayurveda, pharmacopia; plants as source of drugs; Indian medicinal plants and uses - Tulasi, Neem, Pili, Mango, Sarpagandhi, Gulbakavali, Shyma Haldi, Vanchana, Safed Musli, Aswagandha, Satavar, Pipalendi, Digitalis, Senna, Clove, Cardamom, Plantago, *Artemisia annua*, *Coleus forskoli*, Aloe Patal Kumhda, Banpyaz.

(12 Hours)

## **Reference Books:**

- Asutosh Kar, *Medicinal Chemistry*, New Age Publication.
- P. D. Sethi, Dilip Charegaonkar: *Identification of Drugs and Pharmaceutical Formulations by Thin Layer Chromatography* –2nd Edition.
- G.E. Trease, W.C. Evans: *Pharmacognosy*, ELBS.
- Varro E.Tyler, Lynn. R.Brady, James E.Robbers: *Pharmacognosy*.
- T.E. Wallis: *Text Book of Pharmacognosy*, CBS Pub. Delhi.

- Kirthikar, Basu: Indian Medicinal Plants.
- K.M. Nalkarni: Indian Meteria Medica
- W. Dymock: Pharmacographia Indica

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## **DSE – C Lab: Basics of Drug Design & Medicinal Chemistry**

**(60 Hours)**

(a) Drawing of different organic molecules using ChemDraw and ChemSketech software.

(b) Synthesis and characterization of following drugs:

1. Paracetamol,
2. Acetanilide,
3. Aspirin,
4. Phenazone
5. Ibuprofen

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## **DSE – D: Novel Inorganic Solids**

**(Credits: Theory-04, Practicals-02)**  
**Theory: 60 Hours**

### **Unit – 1: Synthesis and modification of inorganic solids**

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

**(10 Hours)**

### **Unit – 2: Inorganic solids of technological importance**

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

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

**(10 Hours)**

### **Unit – 3: Nanomaterials**

Overview of nanostructures and nanomaterials: classification.

Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires. Bio-inorganic nanomaterials, DNA and nanomaterials, natural and antisical nanomaterials, bionano composites.

**(10 Hours)**

#### **Unit – 4: Introduction to engineering materials for mechanical construction**

Composition, mechanical and fabricating characteristics and applications of various types of cast irons, plain carbon and alloy steels, copper, aluminum and their alloys like duralumin, brasses and bronzes cutting tool materials, super alloys thermoplastics, thermosets and composite materials.

**(10 Hours)**

#### **Unit – 5: Composite materials**

Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, environmental effects on composites, applications of composites.

**(10 Hours)**

#### **Unit – 6: Polymers**

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

**(10 Hours)**

#### **Reference Books:**

- Shriver & Atkins. Inorganic Chemistry, Peter Atkins, Tina Overton, Jonathan Rourke, Mark Weller and Fraser Armstrong, 5<sup>th</sup> Edition, Oxford University Press (2011-2012)
- Adam, D.M. Inorganic Solids: An introduction to concepts in solid-state structural chemistry.
- Frank J. Owens, Introduction to Nanotechnology

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#### **DSE – D Lab: Novel Inorganic Solids**

**(60 Hours)**

1. Determination of cation exchange method
2. Determination of total difference of solids.
3. Synthesis of hydrogel by co-precipitation method.
4. Synthesis of silver and gold metal nanoparticles.

#### **Ion exchange:**

- (i) Determination of exchange capacity of cation exchange resins and anion exchange resins.
- (ii) Separation of metal ions from their binary mixture.
- (iii) Separation of amino acids from organic acids by ion exchange chromatography.

**Reference Book:**

- Fahan, *Materials Chemistry*, Springer (2004).
- Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5<sup>th</sup> Ed. The English Language Book Society of Longman.

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**DSE – E: Basic of Polymer Chemistry****(Credits: Theory-04, Practicals-02)****Theory: 60 Hours****Unit – 1: Introduction and Classification**

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

**Functionality and its importance:** Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bi- functional systems, Poly-functional systems.

**(12 Lectures)****Unit – 2: 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)****Unit – 3: Crystallization and crystallinity**

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

**Nature and structure of polymers**-Structure Property relationships.

**(8 Lectures)****Unit – 4: Molecular weight and Glass Transition Temperature of polymers**

(Molecular weight distribution and its significance. Polydispersity index.  $M_n$ ,  $M_w$ , etc) by end group analysis, viscometry, light scattering and osmotic pressure methods.

**Glass transition temperature (T<sub>g</sub>) and determination of T<sub>g</sub>**, Free volume theory, WLF equation, Factors affecting glass transition temperature (T<sub>g</sub>).

**(16 Lectures)****Unit – 5: Polymer Solution**

Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures.

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

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

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

**(16 Lectures)**

#### **Reference 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.
- A Ravve: *Principle of Polymer Chemistry*, Eds. 3<sup>rd</sup>, Springer Science + Business Media, New York, 2012.
- P. Ghosh: *Polymer Science & Technology*, Tata Mcgraw-Hill.
- R.W. Lenz: *Organic Chemistry of Synthetic High Polymers*.

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#### **DSE – E Lab: Basic of Polymer Chemistry**

**(60 Hours)**

##### **1. Polymer synthesis**

- (i) 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-isobutyl-onitrile (AIBN)
- (ii) Preparation of nylon 66/6
- (iii) Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein
  - (a) Preparation of IPC
  - (b) Purification of IPC
  - (c) Interfacial polymerization
- (iv) Redox polymerization of acrylamide
- (v) Precipitation polymerization of acrylonitrile
- (vi) Preparation of urea-formaldehyde resin
- (vii) Preparations of novalac resin/resold resin
- (viii) Microscale Emulsion Polymerization of Poly(methylacrylate)

##### **2. Polymer characterization**

- (i) Determination of molecular weight by viscometry: (a) Polyacrylamide-aq. NaNO<sub>2</sub> solution (b) (Poly vinyl propylidene (PVP) in water

- (ii) Determination of the viscosity-average molecular weight of poly(vinyl alcohol) PVOH) and the fraction of “head-to-head” monomer linkages in the polymer.
- (iii) Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).
- (iv) Testing of mechanical properties of polymers.
- (v) Determination of hydroxyl number of a polymer using colorimetric method.

### 3. Polymer analysis

- (i) Estimation of the amount of HCHO in the given solution by sodium sulphite method
- (ii) Instrumental Techniques
- (iii) IR studies of polymers
- (iv) DSC analysis of polymers
- (v) Preparation of polyacrylamide and its electrophoresis

*\*at least 7 experiments to be carried out.*

### Reference Books:

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

### DSE – F: Green Chemistry

(Credits: Theory-04, Practicals-02)  
Theory: 60 Hours

#### Unit – 1: Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

(4 Hours)

#### Unit – 2: Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/ minimization of hazardous/ toxic products; designing safer chemicals – different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

**(24 Hours)**

### **Unit – 3: Examples of Green Synthesis/ Reactions**

1. Green Synthesis of the following compounds: adipic acid, catechol, BHT, methyl methacrylate, urethane, aromatic amines (4-aminodiphenylamine), benzyl bromide, acetaldehyde, citral, ibuprofen, paracetamol, furfural.
2. Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzoic acid), Oxidation (of toluene, alcohols).
3. Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Orthoester Claisen Rearrangement, Diels-Alder Reaction, Decarboxylation.
4. Microwave assisted solid state reactions: Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles from aldehydes; anhydrides from dicarboxylic acid; pyrimidine and pyridine derivatives; 1,2-dihydrotriazine derivatives; benzimidazoles.
5. Ultrasound assisted reactions: Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizzaro reaction, Strecker synthesis, Reformatsky reaction.

**(16 Hours)**

### **Unit – 4: Future Trends in Green Chemistry**

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; oncovalent derivatization; Green chemistry in sustainable development.

**(8 Hours)**

### **Unit – 5: Green Chemistry in the Fine chemicals and Pharmaceutical Industries**

**(8 Hours)**

#### **Reference Books:**

- V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers (2005).
- P.T. Anastas & J.K. Warner: Oxford Green Chemistry- Theory and Practical, University Press (1998).
- A.S. Matlack: Introduction to Green Chemistry, Marcel Dekker (2001).

- M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
  - M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).
  - Review article from Green Chemistry, Chemical Review.
- 

## DSE – F Lab: Green Chemistry

**60 Hours**

### 1. Safer starting materials

The Vitamin C clock reaction using Vitamin C tablets, tincture of iodine, hydrogen peroxide and liquid laundry starch.

- a) Effect of concentration on clock reaction
- b) Effect of temperature on clock reaction. (if possible)

### 1. Using renewable resources

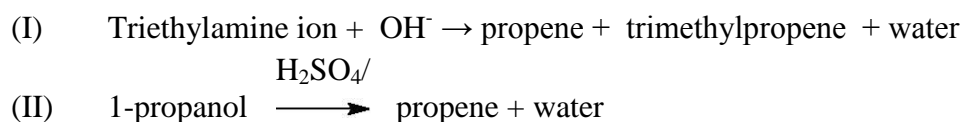
Preparation of biodiesel from vegetable oil.

### 3. Avoiding waste

Principle of atom economy.

Use of molecular model kit to stimulate the reaction to investigate how the atom economy can illustrate Green Chemistry.

Preparation of propene by two methods can be studied



The other types of reactions, like addition, elimination, substitution and rearrangement should also be studied for the calculation of atom economy.

### 4. Use of enzymes as catalysts

Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide  
**Alternative Green solvents**

### 5. Diels Alder reaction in water

Reaction between furan and maleic acid in water and at room temperature rather than in benzene and reflux.

### 6. Environmentally benign extraction of Lycopene from Tomato sauces.

7. Green aqueous Wittig reaction.
8. Microwave assisted Claisen/Dieckman condensation reaction..

#### **Alternative sources of energy**

9. Eosin Y catalyzed visible light Oxidative C-C bond formation reaction.
10. Photo reduction of benzophenone to benzopinacol in the presence of sunlight.

*At least five experiments to be carried out.*

#### **Reference Books:**

- Anastas, P.T & Warner, J.C. *Green Chemistry: Theory and Practice*, Oxford University Press (1998).
- Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).
- Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, Washington DC (2002).
- Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. I.K. *Green Chemistry Experiment: A monograph International Publishing House Pvt Ltd. New Delhi*. Bangalore CISBN 978-93-81141-55-7 (2013).
- Cann, M.C. & Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society (2008).
- Cann, M. C. & Thomas, P. *Real world cases in Green Chemistry*, American Chemical Society (2008).
- Pavia, D. L. Lamponan, G. H. & Kriz, G.S. *W B Introduction to organic laboratory*
- *Journal of Chemical Education* (ACS Publishers) **2014**, 91, 611.
- *Journal of Chemical Education* (ACS Publishers) **2011**, 88, 1014.
- *Journal of Chemical Education* (ACS Publishers) **2000**, 85, 256.

### **DSE – G: Industrial Chemicals and Environment**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Hours**

#### **Unit – 1: Industrial Gases and Inorganic Chemicals**

*Industrial Gases:* Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene.

*Inorganic Chemicals:* Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.

**(10 Hours)**

## **Unit – 2: Industrial Metallurgy**

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

**(4 Hours)**

## **Unit – 3: Environment and its segments**

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

Air Pollution: Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Environmental effects of ozone, Major sources of air pollution.

Pollution by  $\text{SO}_2$ ,  $\text{CO}_2$ ,  $\text{CO}$ ,  $\text{NO}_x$ ,  $\text{H}_2\text{S}$  and other foul smelling gases. Methods of estimation of  $\text{CO}$ ,  $\text{NO}_x$ ,  $\text{SO}_x$  and control procedures.

Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates.

*Water Pollution:* Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems.

Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. Sludge disposal.

Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

**(30 Hours)**

## **Unit – 4: Energy & Environment**

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

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

**(10 Hours)**

## **Unit – 5: Biocatalysis**

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

**(6 Hours)**

## **Reference Books:**

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
- R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley

Publishers, New Delhi.

- J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
  - S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
  - K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
  - S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.
  - S.E. Manahan, *Environmental Chemistry*, CRC Press (2005).
  - G.T. Miller, *Environmental Science* 11th edition. Brooks/ Cole (2006).
  - A. Mishra, *Environmental Studies*. Selective and Scientific Books, New Delhi (2005).
- 

## DSE – G Lab: Industrial Chemicals & Environment

(60 Hours)

1. Determination of dissolved oxygen in water.
2. Determination of Chemical Oxygen Demand (COD)
3. Determination of Biological Oxygen Demand (BOD)
4. Percentage of available chlorine in bleaching powder.
5. Measurement of chloride, sulphate and salinity of water samples by simple titration method ( $\text{AgNO}_3$  and potassium chromate).
6. Estimation of total alkalinity of water samples ( $\text{CO}_3^{2-}$ ,  $\text{HCO}_3^-$ ) using double titration method.
7. Measurement of dissolved  $\text{CO}_2$ .
8. Study of some of the common bio-indicators of pollution.
9. Estimation of SPM in air samples.
10. Preparation of borax/ boric acid.

### Reference Books:

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
  - R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
  - J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
  - S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
  - K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
  - S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.
- 

## DSE – H: Inorganic Materials of Industrial Importance

(Credits: Theory-04, Practicals-02)

Theory: 60 Hours

### Unit – 1: Silicate Industries

*Glass*: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of

glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

*Ceramics:* Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

*Cements:* Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

**(16 Hours)**

## **Unit – 2: Fertilizer**

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

**(8 Hours)**

## **Unit – 3: Surface Coatings**

Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

**(10 Hours)**

## **Unit – 4: Batteries**

Primary and secondary batteries, battery components and their role, Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell.

**(6 Hours)**

## **Unit – 5: Alloys**

Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

**(10 Hours)**

## **Unit – 6: Catalysis & Chemical explosives**

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

Phase transfer catalysts, application of zeolites as catalysts.

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

(10 Hours)

**Reference Books:**

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
- R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
- W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
- J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
- P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
- R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
- B. K. Sharma: *Engineering Chemistry*, Goel Publishing House, Meerut

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**DSE – H Lab: Inorganic Materials of Industrial Importance**

(60 Hours)

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

**Reference Books:**

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
- R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
- W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
- J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
- P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
- R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
- B. K. Sharma: *Engineering Chemistry*, Goel Publishing House, Meerut

**DSE – I: Instrumental Methods of Chemical Analysis**

(Credits: Theory-04, Practicals-02)

Theory: 60 Hours

**Unit – 1: Introduction to spectroscopic methods of analysis**

Recap of the spectroscopic methods covered in detail in the core chemistry syllabus: Treatment of analytical data, including error analysis. Classification of analytical methods and the types of instrumental methods. Consideration of electromagnetic radiation.

**(4 Hours)**

## **Unit – 2: Molecular spectroscopy**

### *Infrared spectroscopy:*

Interactions with molecules: absorption and scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution), advantages of Fourier Transform (FTIR). Samples and results expected. Applications: Issues of quality assurance and quality control, Special problems for portable instrumentation and rapid detection.

*UV-Visible/ Near IR* – emission, absorption, fluorescence and photoacoustic. Excitation sources (lasers, time resolution), wavelength dispersion (gratings, prisms, interference filters, laser, placement of sample relative to dispersion, resolution), Detection of signal (photocells, photomultipliers, diode arrays, sensitivity and S/N), Single and Double Beam instruments, Interpretation (quantification, mixtures, absorption vs. fluorescence and the use of time, photoacoustic, fluorescent tags).

**(16 Hours)**

## **Unit – 3: Separation techniques**

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

### *Immunoassays and DNA techniques*

*Mass spectroscopy:* Making the gaseous molecule into an ion (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, Detection and interpretation (how this is linked to excitation).

**(16 Hours)**

## **Unit – 4: Elemental analysis**

Mass spectrometry (electrical discharges).

Atomic spectroscopy: Atomic absorption, Atomic emission, and Atomic fluorescence.

Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wavelength separation and resolution (dependence on technique), Detection of radiation (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).

**(8 Hours)**

## **Unit – 5:**

**NMR spectroscopy:** Principle, Instrumentation, Factors affecting chemical shift, Spin-coupling, Applications.

**Electroanalytical Methods:** Potentiometry & Voltammetry

Radiochemical Methods

X-ray analysis and electron spectroscopy (surface analysis)

**(16 Hours)**

**Reference books:**

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

**DSE – I Lab: Instrumental Methods of Chemical Analysis**

**(60 Hours)**

1. Safety Practices in the Chemistry Laboratory
2. Determination of the isoelectric pH of a protein.
3. Titration curve of an amino acid.
4. Determination of the void volume of a gel filtration column.
5. Determination of a Mixture of Cobalt and Nickel (UV/Vis spec.)
6. Study of Electronic Transitions in Organic Molecules (i.e., acetone in water)
7. IR Absorption Spectra (Study of Aldehydes and Ketones)
8. Determination of Calcium, Iron, and Copper in Food by Atomic Absorption
9. Quantitative Analysis of Mixtures by Gas Chromatography (i.e., chloroform and carbon tetrachloride)
10. Separation of Carbohydrates by HPLC
11. Determination of Caffeine in Beverages by HPLC Potentiometric Titration of a Chloride-Iodide Mixture
12. Cyclic Voltammetry of the Ferrocyanide/Ferricyanide Couple
13. Nuclear Magnetic Resonance
14. Use of fluorescence to do “presumptive tests” to identify blood or other body fluids.
15. Use of “presumptive tests” for anthrax or cocaine
16. Collection, preservation, and control of blood evidence being used for DNA testing
17. Use of capillary electrophoresis with laser fluorescence detection for nuclear DNA (Y chromosome only or multiple chromosome)
18. Use of sequencing for the analysis of mitochondrial DNA
19. Laboratory analysis to confirm anthrax or cocaine
20. Detection in the field and confirmation in the laboratory of flammable accelerants or explosives

21. Detection of illegal drugs or steroids in athletes
22. Detection of pollutants or illegal dumping
23. Fibre analysis

***At least 10 experiments to be performed.***

#### **Reference Books:**

- Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
- Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.

### **DSE – J: Basic of Nanomaterials**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Hours**

#### **Unit – 1: Introduction and Classification**

What is nanotechnology?; Why nano? Classification of nanostructures, nanoscale architecture; summary of the electronic properties of atoms and solids; the isolated atom, bonding between atoms, giant molecular solids, the free electron model and energy bands of crystalline solids, periodicity of crystal lattices; electronic conduction; effects of the nanometre length scale, changes to the system total energy, changes to the system structure; how nanoscale dimensions affect properties. (electronic conduction, system classification confined to one, two or three dimension and their effect on properties).

**(15 Lectures)**

#### **Unit – 2: Properties of Nanomaterials**

Introductory discussion of size and shape dependable properties of nanomaterials like melting point, magnetism, optical, conductivity (conductor and semi-conductivity), catalytic and electrochemical aspect.

**(10 Lectures)**

#### **Unit – 3: Synthesis of Nanomaterials**

Common methods of top down and bottom approaches of the preparation of nanomaterials. Special interest on the synthesis of metal nanoparticles, metal oxides, and carbon nanotube (CNT) *etc.* A brief discussion of biological synthesis of nanomaterials.

**(10 Lectures)**

#### **Unit – 4: Characterization of Nanomaterials**

A brief historical overview of common instrumental techniques used for characterization of nanomaterials such as, X-ray diffraction, electron microscopy (SEM, TEM, including EDX technique), XPS with respect to working principle, instrumentation and applications. Differential scanning calorimeter (DSC), Thermogravimetric / Differential (TG/DTA), UV-Visible Spectrophotometer, and FTIR –Principle and Applications.

**(15 Lectures)**

#### **Unit – 5: Applications of Nanomaterials**

Use of nanomaterials in daily life with examples (solar cell, GMR read heads, NEMS goniometers, health care, energy materials, *etc*). Societal aspects of nanotechnology: health, environment, hype and reality.

(10 Lectures)

#### Reference Books:

- Hornyak, G. L.; Moore, J. J.; Tibbals, H. F. and Dutta, J. *Fundamentals of Nanotechnology*, CRC Press, 2009.
- Pradeep, T. *A Textbook of Nanoscience and Nanotechnology*, McGraw Hill Edu. New Delhi, (2015).
- Cao, G. *Nanostructures and Nanomaterials Synthesis, Properties and Applications*, Imperial College Press, London, 2004.
- Klabunde, K. J. *Nanoscale materials in Chemistry*, Wiley-Interscience, (2001).
- Knauth, P. and Schoonman, J. *Nanostructured Materials: Selected Synthesis Methods, Properties and Applications*, Kluwer Academic Publishers, New York, (2002).
- Cullity, B. D., *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, **1959**.
- Williams, D. B. and Carter C. B., *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, **1996**.
- Brugel W., in *Introduction to Infrared Spectroscopy*, John Wiley and Sons, New York, **1962**.
- S. Hüfner, in *Photoelectron Spectroscopy: Principles and Applications*, Springer-Verlog, Germany, **1995**.

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#### DSE – J Lab: Basic of Nanomaterials

(60 Hours)

- Verification of the Beer-Lambert law using gold/silver nanoparticles.
- Determination of the band gap of semiconductor nanomaterials.
- Nanochemistry of silver nanoparticles in converting *p*-nitrophenol to *p*-aminophenol.
- Study of surface enhanced Raman scattering activity of silver nanostructures.
- Removal of Mercury by supported nanoparticles.
- Synthesis and characterization of core-shell nanocomposite (bimetallic and oxides)
- Preparation and characterization of nanomaterials by wet chemical routes (sol-gel, reverse micelles, hydrothermal, co-precipitation, *etc.*)

#### Reference Books:

- Pradeep, T. *A Textbook of Nanoscience and Nanotechnology*, McGraw Hill Edu. New Delhi, (2015).

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#### DSE – K : Advanced Organic Chemistry

(Credits: Theory-04, Practicals-02)

Theory: 60 Hours

#### Unit – 1: Nomenclature

Basic nomenclature of bicyclic compounds: Spirocyclic, Polycyclic compounds and heterocyclic compounds.

**(3 Hours)**

## **Unit – 2: Stereochemistry**

Definition of Stereochemistry, Properties of stereoisomers, Tartaric acid and its various isomers, Enantiomeric purity, How do we measure enantiomeric purity, Definition of d.r.; e.r.; ee. Topism, Diastereotopic, Enantiotopic. Prochirality, Making compounds Chiral, Prochiral at sp<sup>2</sup> carbon.

**(10 Hours)**

## **Unit – 3: Reaction Mechanism**

S<sub>N</sub>2, S<sub>N</sub>1 Rate equation, Eyring equation, Linear free Energy relationship. Determining the mechanism of a reaction: Detection and trapping of intermediates, Cross-over experiments, kinetic isotopic effect-primary kinetic and secondary kinetic isotopic effect.

**(7 Hours)**

## **Unit – 4: Introduction of Pericyclic Reaction and Free radical Chemistry**

Definition of Pericyclic reaction. classification of Pericyclic reactions. Cycloaddition reaction (Diels-Alder reaction and its application to the natural products), Sigmatropic rearrangements. Free radical initiation, Barton Reaction, Hoffmann-Löffler-Freytag reaction, Deoxygenation reaction, dehalogenation reaction.

**(10 Hours)**

## **Unit – 5: Functional Group Interconversions**

Functional Groups, Oxidation state, Markonikov-Antimarkonikov addition, Hydration, Acetal/ketal or thioketal formation, Selective reduction, Oxidation of alcohols (Swern oxidation, DMP-oxidation), Stereoselective oxidation and reduction.

**(10 Hours)**

## **Unit – 6: Stereoselective C-C bond formation reaction**

Carbon nucleophile and electrophile, LDA to make enolate, Carbonyl compound reactions, Enolate and pKa, The aldol reaction. Claisen and Dieckmann condensation reaction, Michael addition and Robinson annulations reaction. Acid Promoted reaction (Prins reaction, F-C alkylation and acylation reaction). Benzoin and acylanion equivalent. Retrosynthetic analysis for DA and Robinson annulations reaction.

**(10 Hours)**

## **Unit – 7: NMR Spectroscopy**

Chemical shift, Spin-spin coupling, determining stereochemistry and regiochemistry by <sup>1</sup>H-NMR spectroscopy, <sup>13</sup>C-NMR: 2D NMR COSY, HMBC, HMQC.

**(10 Hours)**

## **References:**

- *Advanced Organic Chemistry* –by J. March 6th Edition
- *Advance Organic Chemistry* (part A) –by A. Carey and R.J. Sundberg
- *Stereochemistry of carbon compound*–by E.L. Eliel
- *Stereochemistry of organic compound*–by Nasipuri
- J. Singh & J.Singh, *Photochemistry and Pericyclic Reactions*,

- W. Carruthers, *Some Modern Methods of Organic Synthesis*, Cambridge University, Press, 1993.
- Bessler and Silverstein, *Spectroscopy of Organic Compounds*, JOHN WILEY, 2001.
- D. C. Pavia, G. M. Lampman, G. S. Kriz, *Introduction to Spectroscopy*, 3<sup>rd</sup> Edition, 2007.
- *Organic Spectroscopy* III Edition—by William Kemp

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## DSE – K Lab: Advanced Organic Chemistry

(60 Hours)

### 1. Hands on experiences:

- To determine the enantiomeric purity (ee/er) by HPLC chromatogram.
- To determine the diastereoisomers ratio from NMR Spectra.
- Analyze the <sup>1</sup>H-NMR Spectra of any organic molecules.
- Analyze the 2D-<sup>13</sup>C-NMR spectra of any organic molecules.

### 2. Synthesis of an Imidazolidinone Organocatalyst and its application in a DA Reaction: Multistep Synthesis.

- Catalyst synthesis
- Diels-Alder reaction.
- Purification step
- Spectral data analysis (<sup>1</sup>H-NMR and <sup>13</sup>C-NMR)

### 3. Robinson annulations

- Two step synthesis of Wieland-Miescher ketone from 1,3-diketone and enones.
- Asymmetric synthesis by chiral proline catalyst
- HPLC Chromatogram and spectral data interpretation.

### 4. Rearrangement of *trans*-stilbene Oxide with Bi(OTf)<sub>3</sub> and other metal triflates.

### 5. Oxidation and Reduction

- Oxidation of secondary alcohol to ketone
- Oxidation of primary alcohol to aldehyde
- Reduction of aldehyde/ketone by NaBH<sub>4</sub>
- Reduction of Ester by using LiAlH<sub>4</sub>

### References:

- Bessler and Silverstein, *Spectroscopy of Organic Compounds*, JOHN WILEY, 2001.
- *J. Chem. Edu.* DOI: 10.1021/acs.jchemed.5b00812
- *J. Chem. Edu.* **2008**, 85, 1531.
- *J. Chem. Edu.* **2011**, 88, 1014.
- *J. Chem. Edu.* **2008**, 85, 1274.
- *Practical Organic Chemistry* by A. I. Vogel.
- *Practical Organic Chemistry* by F. G. Mann and B. C. Saunders.

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## **DSE – L: Research Methodology for Chemistry**

**(Credits: Theory-05, Tutorials-01)**

**Theory: 75 Hours**

### **Unit – 1: 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 Hours)**

### **Unit – 2: 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 Hours)**

### **Unit – 3: 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 Hours)**

### **Unit – 4: 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 Hours)

### Unit – 5: 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 Hours)

### Reference Books

- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) *Practical skills in chemistry*. 2<sup>nd</sup> 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*. 6<sup>th</sup> 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.

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### DSE – L Tutorial: Research Methodology for Chemistry

(Credits: Tutorials-01)

1. Seminar
2. Short Project
3. Literature review

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### DSE – M: Crystalline Material and Properties

(Credits: Theory-05, Tutorials-01)

Theory: 75 Hours

#### Unit – 1: Introduction

Crystalline and non-crystalline solids; space lattice and primitive and non-primitive lattice, crystal structure, unit cell, symmetry in crystal, seven crystal system, Bravais lattice, a qualitative ideas of point and space group; crystal planes and Miller indices, reciprocal lattice. Cubic lattice: lattice point in cubic crystals, coordination number, Packing density, separation between crystal planes

(10 Hours)

#### Unit – 2: Bonding and Crystal Structure of Crystalline Materials

Closed packed structure- hcp and ccp, packing efficiency, voids, limiting radius ratio; description of solid structure of rock salt (NaCl), Wurzite and zinc blend of ZnS, Fluoride (CaF<sub>2</sub>) and antiferite (Na<sub>2</sub>O), Rutile (TiO<sub>2</sub>).

Bonding between atoms in solid: ionic bonds, covalent bonds, metallic bonds, van der Waals bonds; cohesive energy of an ionic crystal, Madelung constant and lattice energy.

(10 Hours)

#### Unit – 3: Determination of Crystal Structure

X-ray diffraction by crystal, Bragg's law, a simple description of rotating crystal method and powder pattern methods. Analysis of powder pattern of simple cubic systems.

A brief overview of determination of crystal structure by electron microscope (TEM, SAED, and HRTEM)

(15 Hours)

#### **Unit – 4: Thermal and Electrical Properties of Solids**

**Thermal Properties:** Specific heat of solids, classical theory – Dulong-Petit's law, Einstein-Debye theory, vibrational modes of one dimensional lattice – dispersion relation and Brillouin zones.

**Electronic Properties:** Free electron theory of metals; solution of one dimensional Schrödinger equation in constant potential; density of state; Fermi energy; Energy band in a solid, explanations of Kronig-Penney model (without derivation), refinement of simple band formation in solid,  $k$ -space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors,  $p$ - $n$  junctions. Hall effect- definition, Hall potential Hall coefficient. Superconductivity- qualitative discussion, critical temperature, Meissner effect, and Josephson Tunnelling.

(15 Hours)

#### **Unit – 5: Magnetic Properties of Solids**

concept of dia- para- and ferro- magnetism; magnetic moment due to orbital and spin motion of electron, effect of temperature, Langevin's theory of dia- and para- magnetism; Curie-Weiss law, qualitative description of ferro-magnetism (magnetic domains), B-H curve, hysteresis loop, retentivity, coercivity, hysteresis loss, soft and hard magnets.

(10Hours)

#### **Reference Books**

- A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
- L. Smart and E. Moore: *Solid State Chemistry*, Chapman and Hall, 1992.
- L. V. Azaroff Introduction to Solid, Tata Mcgraw Hill
- Cullity, B. D., *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, **1959**.
- Williams, D. B. and Carter C. B., *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, **1996**.

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#### **DSE – M Tutorial: Crystalline Material and Properties**

(Credits: Tutorials-01)

- Indexing of powder XRD pattern and calculation of lattice parameter for crystals.
- Analyzing of TEM images and Indexing of SAED pattern and HRTEM images.

#### **Reference Books**

- Cullity, B. D., *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, **1959**.
- Williams, D. B. and Carter C. B., *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, **1996**.

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#### **DSE – N: Basic Mathematical Concept for Chemist**

Credits: Theory-05, Tutorial-01)

(75 Hours)

### Unit – 1: Logarithmic Relations, Numbers, and Vectors

**Logarithmic Relations. Numbers;** Real and Complex number.

**Vectors:** Vectors, dot, cross and triple product etc. The gradient, divergence and curl. Vector calculus, Gauss' theorem, divergence theorem *etc.*

(15 Hours)

### Unit – 2: Matrix Algebra

Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (symmetric, screw-symmetric, Hermitian, screw-Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations; homogeneous, non-homogeneous linear equation and conditions for the solution, linear dependence and independence. Introduction of vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants.

(15 Hours)

### Unit – 3: Differential and Calculus

**Differential:** Functions, continuity and differentiability, rules for differentiation, application of differential calculus including maxima and minima, exact and inexact differentials, their application to related to chemistry syllabus.

**Partial Differential:** Function of several variables, partial differentiation, co-ordinate transformation (e.g. Cartesian to spherical polar).

**Integral calculus:** Basic rules for integration, integration by parts, partial fraction and substitution, reduction formulae, applications of integral calculus.

(15 Hours)

### Unit – 4: Elementary Differential Equations

Ordinary first- and second-order differential equations. Partial differential equations. Solution of inexact differential equations by the method of integrating factors. Power series and extended power series solutions.

(15 Hours)

### Unit – 5: Probability and Curve Sketching

Permutation & Combination. Factorial and probability. Curve sketching linear graphs and calculation of slopes, and curve fitting.

(15 Hours)

### Reference Books:

- The Chemistry Maths Book, Oxford University Press, New Delhi (2011)
- R. G. Mortimer: *Mathematics for Physical Chemistry*, Academic Press
- F. Diniels: *Mathematical Preparation for Physical chemistry*, McGraw Hill.

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### DSE – N Tutorial: Basic Mathematical Concept for Chemistry

(Credits: Tutorials-01)

- Solving numerical problems related to chemistry syllabus especially related to quantum mechanics, thermodynamics, kinetics etc.

**\*\*Skill Enhancement Course (SEC) in Chemistry**  
**Skill Enhancement Course (any two) (Credit: 04 each)- SEC1 to SEC2**

**CHM T 214 and CHM T 224**

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**SEC – A: IT Skill for Chemists**

**(Credits: 04)**

**Theory: 60 Hours**

**Unit – 1: Mathematics**

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

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

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

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

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

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

**(10 Hours)**

**Unit – 2: Computer programming**

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

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

**(10 Hours)**

## HANDS ON

### Unit – 3: Introductory writing activities

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

(10 Hours)

### Unit – 4: Handling numeric data

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

(10 Hours)

### Unit – 5: Numeric modeling

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

(10 Hours)

### Unit – 6: Statistical analysis

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

**Presentation:** Presentation graphics

(10 Hours)

### Reference Books:

- McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
- Mortimer, R. Mathematics for Physical Chemistry. 3<sup>rd</sup> Ed. Elsevier (2005).
- Steiner, E. The Chemical Maths Book Oxford University Press (1996).
- Yates, P. Chemical calculations. 2<sup>nd</sup> Ed. CRC Press (2007).
- Harris, D. C. *Quantitative Chemical Analysis*. 6<sup>th</sup> 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.
- Noggle, J. H. *Physical chemistry on a Microcomputer*. Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).

## SEC – B: Basic Analytical Chemistry

(Credits: 04)  
Theory: 60 Hours

### Unit – 1: 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.

(10 Hours)

### Unit – 2: Volumetric Titration

Standard solution, primary standard and secondary standard, titration, end point, indicator, concentration of standard solution- moles, Normality, molarity, Molality, parts per million (PPM), volumetric calculation, acid base titration and use of indicators, titration curves for strong acid vs strong base, weak acid with strong base, weak base with strong acid, theory of acid base indicator, Redox titration- titration of Mohr salt against  $\text{KMnO}_4$ , Titration of Oxalic acid against  $\text{KMnO}_4$ , Titration of  $\text{FeSO}_4$  against  $\text{K}_2\text{Cr}_2\text{O}_7$ , Iodometric and iodimetric titration, Internal and external indicator, complexometric titration- EDTA titration, Eriochrome black T indicator, complexometric titration curve, direct and back titration, masking and demasking of cations, precaution in volumetric titration.

(15 Hours)

### Unit – 3: Qualitative Analysis of Inorganic Radicals

Introduction to salt analysis, dry and wet test for acid and basic radicals, Principle and chemistry of qualitative analysis of inorganic salt; chemistry involved in qualitative analysis of mixture containing interfering radicals and insolubles.

(10 Hours)

### Unit – 3: Chromatography

Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.

- Paper chromatographic separation of mixture of metal ion ( $\text{Fe}^{3+}$  and  $\text{Al}^{3+}$ ).
- To compare paint samples by TLC method.

**Solvent Extraction:** Distribution Coefficient, distribution ratio, percent extracted, solvent extraction of metals ions, extraction of ion association complex, extraction of metal chelates, multiple batch extraction and applications.

**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).

(10 Hours)

### Unit – 4: Suggested Applications (Any one):

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

(5 Hours)

### Unit – 5: 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.

**(10 Hours)**

#### Reference Books:

1. Willard, H. H. *Instrumental Methods of Analysis*, CBS Publishers.
2. Skoog & Lerry. *Instrumental Methods of Analysis*, Saunders College Publications, New York.
3. Skoog, D.A.; West, D.M. & Holler, F.J. *Fundamentals of Analytical Chemistry 6<sup>th</sup> Ed.*, Saunders College Publishing, Fort Worth (1992).
4. Harris, D. C. *Quantitative Chemical Analysis*, W. H. Freeman.
5. Dean, J. A. *Analytical Chemistry Notebook*, McGraw Hill.
6. Day, R. A. & Underwood, A. L. *Quantitative Analysis*, Prentice Hall of India.
7. Freifelder, D. *Physical Biochemistry 2<sup>nd</sup> Ed.*, W.H. Freeman and Co., N.Y. USA (1982).
8. Cooper, T.G. *The Tools of Biochemistry*, John Wiley and Sons, N.Y. USA. 16 (1977).
9. Vogel, A. I. *Vogel's Qualitative Inorganic Analysis 7<sup>th</sup> Ed.*, Prentice Hall.
10. Vogel, A. I. *Vogel's Quantitative Chemical Analysis 6<sup>th</sup> Ed.*, Prentice Hall.
11. Robinson, J.W. *Undergraduate Instrumental Analysis 5<sup>th</sup> Ed.*, Marcel Dekker, Inc., New York (1995).

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### SEC – C: Chemical Technology & Environmental Aspects for Society

**(Credits: 04)**

**Theory: 60 Hours**

#### Unit – 1: Chemical Technology

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

**(20 Hours)**

#### Unit – 2: Society

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

combustion to complex instances like genetic engineering and the manufacture of drugs.

**(20 Hours)**

### **Unit – 3: Uses of Hazard Chemical in Laboratory**

Sodium metal, Sodium Azide, Grignard reagent, Concentrated H<sub>2</sub>SO<sub>4</sub>, HNO<sub>3</sub> & HCl, Arsenic oxide,

**(10 Hours)**

### **Unit – 4: Effect of Disposal Materials from Industry**

Waste water, Skin effect, Fertilizer activity of Soil, Impact of polythene in river or Ocean etc.

**(10 Hours)**

### **Reference Book:**

- John W. Hill, Terry W. McCreary & Doris K. Kolb, *Chemistry for changing times* 13<sup>th</sup> Ed.
  - A. K. Dey, Environmental Chemistry
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## **SEC – D: Cheminformatics**

**(Credits: 04)**

**Theory: 60 Hours**

### **Unit – 1: Introduction to Chemoinformatics**

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

**(10 Hours)**

### **Unit – 2: Representation of molecules and chemical reactions**

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

**(10 Hours)**

### **Unit – 3: Searching chemical structures**

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

**(10 Hours)**

### **Unit – 4: Applications**

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

**(20 Hours)**

#### **Unit – 5: Hands-on Exercises**

**(10 Hours)**

#### **Reference Books:**

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

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### **SEC – E: Green Methods in Chemistry**

**(Credits: 04)**

**Theory: 60 Hours**

#### **Unit – 1: Short Introduction to Green Chemistry**

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

**(10 Hours)**

#### **Unit – 2: Principles**

Tools of Green chemistry, Twelve principles of Green Chemistry, with examples.

**(10 Hours)**

#### **Unit – 3: Prevention of Byproducts**

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

- 1 A green synthesis of ibuprofen which creates less waste and fewer byproducts (Atom economy).
- 2 Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments.
- 3 Environmentally safe antifoulant.
- 4 CO<sub>2</sub> as an environmentally friendly blowing agent for the polystyrene foam sheet packaging market.
- 5 Using a catalyst to improve the delignifying (bleaching) activity of hydrogen

- peroxide.
- 6 A new generation of environmentally advanced preservative: getting the chromium and arsenic out of pressure treated wood.
  - 7 Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
  - 8 Development of a fully recyclable carpet: cradle to cradle carpeting.

**(40 Hours)**

#### **Reference Books:**

1. Manahan S.E. (2005) Environmental Chemistry, CRC Press
2. Miller, G.T. (2006) Environmental Science 11th edition. Brooks/Cole
3. Mishra, A. (2005) Environmental Studies. Selective and Scientific Books, New

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### **SEC – F: Cosmetics, Perfumes & Pharmaceutical Chemistry**

**(Credits: 04)**

**Theory: 60 Hours**

#### **Unit – 1: Introduction of Cosmetics & perfumes chemistry**

History of Cosmetics & perfumes chemistry, a general study including preparation and uses of the following: Hair dye, hair spray, shampoo, suntan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone.

**(20 Hours)**

#### **Unit – 2: Synthesis procedure**

1. Preparation of talcum powder.
2. Preparation of shampoo.
3. Preparation of enamels.
4. Preparation of hair remover.
5. Preparation of face cream.
6. Preparation of nail polish and nail polish remover.

**(10 Hours)**

#### **Unit – 3: Drugs & Pharmaceuticals**

Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-

inflammatory agents (Aspirin, paracetamol, Ibuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

**(20 Hours)**

#### **Unit – 4: 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.

**(10 Hours)**

#### **Reference 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.
  - 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.
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### **SEC – G: Pesticide & Fuel Chemistry**

**(Credits: 04)**

**Theory: 60 Hours**

#### **Unit – 1: Introduction of Pesticide Chemistry & Preparation Procedure**

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).

**(20 Hours)**

#### **Unit – 2: Introduction and Industrial Manufacture of Fuel Energy Sources**

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 based 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.

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, pour point) and their determination.

**(40 Hours)**

**Reference 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.

**Reference Book:**

- R. Cremllyn: *Pesticides*, John Wiley.

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**SEC – H: Computer Science/Sports/NCC/NSS/Yoga etc. offered by respective Department**

**(Credits: 04)**

**Theory: 60 Hours**

**\*Course Structure for SEC – H to be offered by respective Department**

## Generic Elective Course (GE) (Minor-Chemistry) (any four) for other Departments/Disciplines:

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**GE – A: Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Hours**

**Section – A: Inorganic Chemistry – 1**

### **Unit – 1: Atomic Structure**

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

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

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

**(12 Hours)**

### **Unit – 2: Chemical Bonding**

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

*Covalent bonding:* VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements, such as  $\text{BeCl}_2$ ,  $\text{BF}_3$ ,  $\text{SiF}_4$ ,  $\text{PCl}_5$ ,  $\text{SF}_6$ ,  $\text{NH}_3$ ,  $\text{H}_2\text{O}$ ,  $\text{OF}_2$ ,  $\text{ClF}_3$ ,  $\text{SF}_4$ ,  $\text{XeF}_4$ ,  $\text{XeF}_6$ ,  $\text{H}_3\text{O}^+$ ,  $\text{I}_3^-$ ,  $\text{I}_3^+$ ,  $\text{ICl}_2^-$ ,  $\text{XeF}_5^+$ .

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

**(10Hours)**

### Unit – 3: Molecular Orbital Theory

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

(8 Hours)

### Section – B: Organic Chemistry – I

#### Unit – 1: Fundamentals of Organic Chemistry

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis.

Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals.

Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule.

(8 Hours)

#### Unit – 2: Stereochemistry

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

(10 Hours)

#### Unit – 3: Aliphatic Hydrocarbons

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

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

**Alkenes:** (Upto 5 Carbons) *Preparation:* Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); *cis* alkenes (Partial catalytic hydrogenation) and *trans* alkenes (Birch reduction). *Reactions:* *cis*-addition (alk. KMnO<sub>4</sub>) and *trans*-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymercuration-demercuration, Hydroboration-oxidation.

**Alkynes:** (Upto 5 Carbons) *Preparation:* Acetylene from CaC<sub>2</sub> and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides.

*Reactions:* formation of metal acetylides, addition of bromine and alkaline  $\text{KMnO}_4$ , ozonolysis and oxidation with hot alk.  $\text{KMnO}_4$ .

**(12 Hours)**

**Reference Books:**

- J. D. Lee: *A new Concise Inorganic Chemistry*, E L. B. S.
- F. A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
- Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
- James E. Huheey, Ellen Keiter and Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
- T. W. Graham Solomon: *Organic Chemistry*, John Wiley and Sons.
- Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
- E. L. Eliel: *Stereochemistry of Carbon Compounds*, Tata McGraw Hill.
- I. L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
- R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
- Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand

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**GE – A Lab: Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons**

**(60 Hours)**

***Section – A: Inorganic Chemistry - Volumetric Analysis***

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with  $\text{KMnO}_4$ .
3. Estimation of water of crystallization in Mohr's salt by titrating with  $\text{KMnO}_4$ .
4. Estimation of Fe (II) ions by titrating it with  $\text{K}_2\text{Cr}_2\text{O}_7$  using internal indicator.
5. Estimation of Cu (II) ions iodometrically using  $\text{Na}_2\text{S}_2\text{O}_3$ .

***Section – B: Organic Chemistry***

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

**Reference Books:**

- Textbook of Practical Organic Chemistry, A.I. Vogel , Prentice Hall, 5th edition.
  - Practical Organic Chemistry, F. G. Mann. & B. C. Saunders, Orient Longman, 1960.
  - Vogel's Qualitative Inorganic Analysis, A.I. Vogel, Prentice Hall, 7th Edition.
  - Vogel's Quantitative Chemical Analysis, A.I. Vogel, Prentice Hall, 6th Edition.
  - A. K. Nad, B. Mahapatra and A. Ghosal, An Advanced Course in Practical Chemistry, New Central Book Agency Priv. Ltd, 2011
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## **GE – B: Kinetic Theory of Gases, Chemical Energetics, Equilibria & Functional Group Organic Chemistry**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Hours**

### ***Section – A: Physical Chemistry – I***

#### **Unit – 1: Kinetic Theory of Gases**

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

Deviation of real gases from ideal behaviour, compressibility factor, causes of deviation. van der Waals equation of state for real gases. Boyle temperature (derivation not required). Critical phenomena, critical constants and their calculation from van der Waals equation. Andrews isotherms of CO<sub>2</sub>.

Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation – derivation not required) and their importance.

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

**(10 Hours)**

#### **Unit – 2: Chemical Energetics**

**Chemical Energetics:** Introduction of different terms and processes in thermodynamics: [systems (isolated, closed, open) and surrounding, macroscopic properties, state and path functions and their differentials.

**First Law:** concept of heat,  $q$ , work,  $w$ , internal energy,  $U$ , sign convention for heat and work, nature of work, path dependence of work and heat; statement of first law; enthalpy,  $H$ , heat changes at constant volume and constant pressure; heat capacities ( $C_v$ ,  $C_p$ ) and relation between them for ideal gases. Reversible and irreversible processes, maximum work, thermodynamic quantities ( $w$ ,  $q$ ,  $\Delta U$ ,  $\Delta H$ ) and its calculation for isothermal and adiabatic reversible expansion of ideal gases. Ideal gas law for adiabatic reversible expansion, comparison of adiabatic and isothermal reversible expansion. Joule-Thomson effect, Joule-Thomson coefficient in ideal and real (van der Waal) gases, inversion temperature.

**Thermo-chemistry:** Standard state, standard enthalpy of formation, Hess's Laws of constant heat summation and its application. Change in internal energy ( $\Delta U$ ) and enthalpy ( $\Delta H$ ) of chemical reactions, relation between  $\Delta U$  and  $\Delta H$ , variation of heat of reaction with temperature (Kirchhoff's equation). Enthalpy of neutralization. Bond Energy – Bond dissociation energy and its calculation from thermo-chemical data.– Kirchhoff's equation.

Second law of thermodynamics, concept of entropy, free energy work functions, Gibbs Helmholtz equation and its applications

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

(12 Hours)

### Unit – 3: Chemical and Ionic Equilibrium

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

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

(8 Hours)

### Section – B: Organic Chemistry – 2

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

### Unit – 1: Aromatic Hydrocarbons & Alkyl and Aryl Halides

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

**Alkyl Halides (upto 5 Carbons):** Types of Nucleophilic Substitution ( $S_N2$ ,  $S_N1$ ,  $S_Ni$ ) reactions. *Preparation:* from alkenes and alcohols. *Reactions:* hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation. Williamson's ether synthesis: Elimination vs substitution.

**Aryl Halides:** *Preparation:* (Chloro, bromo and iodo-benzene case): from phenol, Sandmeyer & Gattermann reactions. *Reactions (Chlorobenzene):* Aromatic nucleophilic substitution (replacement by  $-OH$  group) and effect of nitro substituent. Benzyne Mechanism:

KNH<sub>2</sub>/NH<sub>3</sub> or NaNH<sub>2</sub>/NH<sub>3</sub> reagent system. Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

(10 Hours)

## Unit – 2: Alcohols, Phenols, Ethers, Aldehydes and Ketones (Upto 5 Carbons)

**Alcohols:** *Preparation:* Preparation of 1°, 2° and 3° alcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters. *Reactions:* With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. KMnO<sub>4</sub>, acidic dichromate, conc.HNO<sub>3</sub>). Oppeneauer oxidation *Diols:* (Upto 6 Carbons) oxidation of diols. Pinacol-Pinacolone rearrangement.

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

**Ethers (Aliphatic and Aromatic):** Cleavage of ethers with HI.

**Aldehydes and Ketones (Aliphatic and Aromatic):** (Formaldehyde, acetaldehyde, acetone and benzaldehyde); *Preparation:* from acid chlorides and from nitriles. *Reactions* -Reaction with HCN, ROH, NaHSO<sub>3</sub>, NH-G derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Ponndorf Verley reduction.

(12 Hours)

## Unit – 3: Carboxylic acids and their derivatives & Amines salt

**Carboxylic acids (aliphatic and aromatic):** *Preparation:* Acidic and Alkaline hydrolysis of esters. *Reactions:* Hell – Vohlard - Zelinsky Reaction. *Preparation:* Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversion. *Reactions:* Comparative study of nucleophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation.

**Amines and Diazonium Salts:** Amines (Aliphatic and Aromatic): (Upto 5 carbons), *Preparation:* from alkyl halides, Gabriel's Phthalimide synthesis, Hofmann Bromamide reaction. *Reactions:* Hofmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, with HNO<sub>2</sub>, Schotten – Baumann Reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation.

**Diazonium salts:** *Preparation:* from aromatic amines. *Reactions:* conversion to benzene, phenol, dyes.

(8 Hours)

## Reference Books:

- T. W. Graham Solomons: *Organic Chemistry, John Wiley and Sons.*
- Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry, Orient Longman.*
- R. T. Morrison & R. N. Boyd: *Organic Chemistry, Prentice Hall.*
- Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry, S. Chand.*

- G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).
  - G. W. Castellan: *Physical Chemistry* 4th Edn. Narosa (2004).
  - J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
  - 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)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
  - B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).
  - R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
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## **GE – B Lab: Kinetic Theory of Gases, Chemical Energetics, Equilibria & Functional Group Organic Chemistry**

**(60 Hours)**  
**(Practicals : 02)**

### ***Section – A: Physical Chemistry***

#### **Thermochemistry**

1. Determination of heat capacity of calorimeter for different volumes.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Determination of enthalpy of ionization of acetic acid.
4. Determination of integral enthalpy of solution of salts ( $\text{KNO}_3$ ,  $\text{NH}_4\text{Cl}$ ).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of  $H$ .

#### **Ionic Equilibria**

##### **pH measurements**

- a) Measurement of pH of different solutions like aerated drinks, fruit juices, shampoos and soaps (use dilute solutions of soaps and shampoos to prevent damage to the glass electrode) using pH-meter.
- b) Preparation of buffer solutions:
  - (i) Sodium acetate-acetic acid
  - (ii) Ammonium chloride-ammonium hydroxide

Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

### ***Section – B: Organic Chemistry***

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

## **II**

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

### **Reference Books**

- A.I. Vogel: Textbook of Practical Organic Chemistry, 5th edition, Prentice-Hall.
  - F. G. Mann & B. C. Saunders, Practical Organic Chemistry, Orient Longman (1960).
  - Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press
  - B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.
  - A. K. Nad, B. Mahapatra and A. Ghosal, An Advanced Course in Practical Chemistry, New Central Book Agency Priv. Ltd, 2011
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### **GE – C: Solid, Solutions, Phase Equilibrium, Conductance, Periodic Properties and Chemistry of s-, p-, and d- block elements**

**(Credits: Theory-04, Practicals-02)**  
**Theory: 60 Hours**

#### ***Section – A: Physical Chemistry – 2***

#### **Unit – 1: Solids**

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

**(10 Hours)**

#### **Unit – 2: Solutions & Phase Equilibrium**

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

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

Phases, components and degrees of freedom of a system, criteria of phase equilibrium. Gibbs Phase Rule and its thermodynamic derivation. Derivation of Clausius – Clapeyron equation and its importance in phase equilibria. Phase diagrams of one-component systems (water and sulphur) and two component systems involving eutectics, congruent and incongruent melting points (lead-silver,  $\text{FeCl}_3\text{-H}_2\text{O}$  and Na-K only).

**(12 Hours)**

### **Unit – 3: Conductance**

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch law of independent migration of ions.

Transference number and its experimental determination using Hittorf and Moving boundary methods. Ionic mobility. Applications of conductance measurements: determination of degree of ionization of weak electrolyte, solubility and solubility products of sparingly soluble salts, ionic product of water, hydrolysis constant of a salt. Conductometric titrations (only acid-base).

**(8 Hours)**

### **Section – B: Inorganic Chemistry – 2**

#### **Unit – 1: Periodic Properties & Acid-Base Concepts**

**Periodic Properties:** Division of elements into *s*, *p*, *d*, and *f* blocks, covalent radii, van der Waals radii and ionic radii; ionization enthalpy, electron gain enthalpy, and electronegativity (Pauling, Mulliken, and Alfred-Rochow scales: Definition, methods of determination, trends in periodic table, and applications in predicting and explaining chemical behavior).

**Acids and Bases:** Arrhenius, Brønsted-Lowry, Lux-Flood and Lewis concepts of acids and bases. Factors affecting strengths of Lewis acids and bases, Classification of acids and bases as hard and soft, Pearsons HSAB concept, acid-base strength and hardness and softness, symbiosis, application of HSAB theory.

**(10 Hours)**

#### **Unit – 2: Oxidation-Reduction**

Redox equations, Standard electrode potentials, Ellingham diagrams for reduction of metal oxides using carbon as reducing agent, Nernst equation, redox potentials to explore the feasibility of reaction and calculation of values of equilibrium constant,

**(6 Hours)**

#### **Unit – 3: Chemistry of *s*-, *p*- and *d*- Block Elements**

**s-Block Elements:** General characteristic properties, complexes of alkali metals, comparative study of hydrides, oxides, hydroxides, halides, carbonates and bicarbonates of group I and II, Diagonal relationship, Biological role of alkali and alkaline earth metals.

**p-Block Elements:** General characteristic properties, comparative study (including diagonal relationship and inert pair effect) of groups 13-17 (B, C, N, O, F) elements and group trends of compounds like hydrides, oxides, halides, and oxy acids; preparation properties and structure, of diborane, borazine, alkalimetal borohydrides, fullerenes, silicates and silicones, inter-halogens and polyhalides.

**Chemistry of Noble Gases:** Isolation and separation of noble gases from air, chemical properties of noble gases, chemistry of xenon, structure and bonding in xenon compounds.

**d-Block Elements:** Characteristic properties of d-block elements. Properties of the elements of the first transition series, their binary compounds and complexes illustrating relative stability of their oxidation states, coordination number and geometry. Comparative treatment with their 3d-analogues in respect of ionic radii, oxidation states and stereochemistry.

(14 Hours)

#### Reference Books:

- G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).
- G. W. Castellan: *Physical Chemistry* 4th Ed. Narosa (2004).
- J. C. Kotz, P. M. Treichel, J. R. Townsend, *General Chemistry*, Cengage Learning India Pvt. Ltd.: New Delhi (2009).
- B. H. Mahan: *University Chemistry*, 3rd Edn. Narosa (1998).
- R. H. Petrucci, *General Chemistry*, 5th Edn., Macmillan Publishing Co.: New York (1985).
- E. S. Gilreath, *Fundamental Concepts of Inorganic Chemistry*, Mc Graw Hill Edu. Pvt. Ltd.
- R. Sarkar (Part-I & II), *General & Inorganic Chemistry*, Central.
- R. L. Dutta (Part-I & II), *Inorganic Chemistry*, The New Book Stall.
- J. D. Lee: *A New Concise Inorganic Chemistry*, E.L.B.S.
- F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
- D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
- Gary Wulfsberg: *Inorganic Chemistry*, Viva Books Pvt. Ltd.

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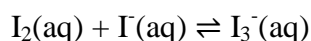
#### GE – C Lab: Solid, Solutions, Phase Equilibrium, Conductance & Periodic Properties and Chemistry of s-, p-, and d- block elements

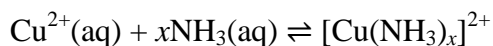
(60 Hours)

##### Section – A: Physical Chemistry

##### Distribution

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





### Phase equilibria

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

### Conductance

- Determination of cell constant
- Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
- Perform the following conductometric titrations:
  - Strong acid vs. strong base
  - Weak acid vs. strong base

### Potentiometry

Perform the following potentiometric titrations:

- Strong acid vs. strong base
- Weak acid vs. strong base
- Potassium dichromate vs. Mohr's salt

### Section – B: Inorganic Chemistry

Semi-micro qualitative analysis using  $\text{H}_2\text{S}$  of mixtures- not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

Cations :  $\text{NH}_4^+$ ,  $\text{Pb}^{2+}$ ,  $\text{Ag}^+$ ,  $\text{Bi}^{3+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Sn}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$ ,  $\text{Co}^{2+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{K}^+$ , Anions :  $\text{CO}_3^{2-}$ ,  $\text{S}^{2-}$ ,  $\text{SO}_3^{2-}$ ,  $\text{S}_2\text{O}_3^{2-}$ ,  $\text{NO}_3^-$ ,  $\text{NO}_2^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{PO}_4^{3-}$ ,  $\text{BO}_3^{3-}$ ,  $\text{C}_2\text{O}_4^{2-}$ ,  $\text{F}^-$

*(Spot tests should be carried out wherever feasible)*

### Reference Books:

- B.D. Khosla: Senior Practical Physical Chemistry, R. Chand & Co.
- A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- A.I. Vogel, Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- A. K. Nad, B. Mahapatra and A. Ghosal, An Advanced Course in Practical Chemistry, New Central Book Agency Priv. Ltd, 2011
- V. K. Ahluwalia, S. Dhingra & A. Gulati, College Practical Chemistry, University Press, Delhi.

**GE – D: Electrochemistry, Chemical Kinetics, Co-ordination compounds,  
Organometallics and Molecules of life**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Hours**

***Section – A: Physical Chemistry – 3***

**Unit – 1: Electrochemistry**

Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell. Nernst equation and its importance. Types of electrodes. Standard electrode potential. Electrochemical series. Thermodynamics of a reversible cell, calculation of thermodynamic properties:  $G$ ,  $H$  and  $S$  from EMF data. Calculation of equilibrium constant from EMF data. pH determination using hydrogen electrode and glass electrode. Potentiometric titrations -qualitative treatment (acid-base and oxidation-reduction only).

**(10 Hours)**

**Unit – 2: Chemical Kinetics**

The concept of reaction rates. Effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction. Derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants). Half-life of a reaction. General methods for determination of order of a reaction. Concept of activation energy and its calculation from Arrhenius equation.

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

**(10 Hours)**

***Section – B: Inorganic Chemistry – 3***

**Unit – 1: Coordination Compounds**

Werner's coordination theory and its experimental verification, effective atomic number concept, chelates, nomenclature of co-ordination compounds, isomerism in coordination compounds.

**Crystal Field Theory:** Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors affecting the magnitude of  $\Delta$ . Spectrochemical series. Comparison of CFSE for  $O_h$  and  $T_d$  complexes, Tetragonal distortion of octahedral geometry. Jahn-Teller distortion, Square planar coordination.

**(10 Hours)**

**Unit – 2: Organometallics**

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

(10 Hours)

### **Section – C: Organic Chemistry – 3**

#### ***Molecules of Life***

##### **Unit – 1: Carbohydrates**

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

(8 Hours)

##### **Unit – 2: Amino Acids, Peptides, Proteins and Nucleic Acids**

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

*Reactions of Amino acids:* ester of  $-\text{COOH}$  group, acetylation of  $-\text{NH}_2$  group, complexation with  $\text{Cu}^{2+}$  ions, ninhydrin test.

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

Components of Nucleic acids: Adenine, guanine, thymine and Cytosine (Structure only), other components of nucleic acids, Nucleosides and nucleotides (**nomenclature**), Structure of polynucleotides; Structure of DNA (Watson-Crick model) and RNA(**types of RNA**), Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation.

(12 Hours)

#### **Reference Books:**

- G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).
- G. W. Castellan: *Physical Chemistry* 4th Edn. Narosa (2004).
- J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
- B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).

- R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
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- F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
- D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
- R. L. Dutta (Part-I & II), *Inorganic Chemistry*, The New Book Stall.
- Gary Wulfsberg: *Inorganic Chemistry*, Viva Books Pvt. Ltd.
- S. Chand. 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)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Biochemistry* 7<sup>th</sup> Ed., W. H. Freeman.
- Berg, J. M., Tymoczko, J. L. & Stryer, L. *Biochemistry* 7<sup>th</sup> Ed., W. H. Freeman

**GE – D Lab: Electrochemistry, Chemical Kinetics, Co-ordination compounds,  
Organometallics and Molecules of life**

**(60 Hours)**

**Section – A: Physical Chemistry**

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

- a) Determination of the surface tension of a liquid or a dilute solution using a stalagmometer.
- b) Study of the variation of surface tension of a detergent solution with concentration.

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

- a) Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwald's viscometer.
- b) Study of the variation of viscosity of an aqueous solution with concentration of solute.

(III) Chemical Kinetics

Study the kinetics of the following reactions.

1. Initial rate method: Iodide-persulphate reaction
3. Integrated rate method:
  - c. Acid hydrolysis of methyl acetate with hydrochloric acid.
  - b. Saponification of ethyl acetate.
  - c. Compare the strengths of HCl and H<sub>2</sub>SO<sub>4</sub> by studying kinetics of hydrolysis of methyl acetate

### ***Section – B: Inorganic Chemistry***

1. Separation of mixtures by chromatography: Measure the  $R_f$  value in each case.  
(Combination of two ions to be given)  
Binary mixture of nickel and cobalt, copper and nickel, zinc and magnesium, iron and copper; aluminium and nickel.
2. Preparation of any two of the following complexes:
  - (a) tetraammine copper (II) sulphate
  - (b) tetraamminecarbonatocobalt (III) nitrate
  - (c) potassium trioxalatochromate (III)
  - (d) potassium trioxalatoferrate (III)
  - (e) sodium hexanitritocobaltate (III)
  - (f) prussian blue

### ***Section – C: Organic Chemistry***

1. Determination of the concentration of glycine solution by formylation method.
2. Titration curve of glycine
3. Action of salivary amylase on starch
4. Effect of temperature on the action of salivary amylase on starch.
5. Determination of the saponification value of an oil/fat.
6. Determination of the iodine value of an oil/fat
7. Differentiation between a reducing/nonreducing sugar.
8. Extraction of DNA from onion/ cauliflower

#### **Reference Books:**

- B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.
- A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- A.I. Vogel, Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- A. K. Nad, B. Mahapatra and A. Ghosal, An Advanced Course in Practical Chemistry, New Central Book Agency Priv. Ltd, 2011
- V. K. Ahluwalia, S. Dhingra & A. Gulati, College Practical Chemistry, University Press, Delhi.

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### **GE – E: Analytical Chemistry, Quantum Chemistry & Spectroscopy**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Hours**

#### ***Section – A: Inorganic Chemistry – 4***

#### **Unit – 1: Introduction**

Introduction to Analytical Chemistry and its interdisciplinary nature. Balances, burettes, volumetric flasks, pipettes, calibration of tools, sampling. Errors and Statistics: significant figures, rounding off, accuracy and precision, determinate and indeterminate errors, standard deviation, propagation of errors, confidence limit, test of significance, rejection of a result.

(8 Hours)

### Unit – 2: Volumetric Titration

Standard solution, primary standard and secondary standard, titration, end point, indicator, concentration of standard solution- moles, Normality, molarity, Molality, parts per million (PPM), volumetric calculation, acid base titration and use of indicators, titration curves for strong acid vs strong base, weak acid with strong base, weak base with strong acid, theory of acid base indicator, Redox titration- titration of Mohr salt against  $\text{KMnO}_4$ , Titration of Oxalic acid against  $\text{KMnO}_4$ , Titration of  $\text{FeSO}_4$  against  $\text{K}_2\text{Cr}_2\text{O}_7$ , Iodometric and iodimetric titration, Internal and external indicator, complexometric titration- EDTA titration, Eriochrome black T indicator, complexometric titration curve, direct and back titration, masking and demasking of cations, precaution in volumetric titration and Gravimetric methods.

(10 Hours)

### Unit – 3: Chromatography

**Chromatographic Techniques:** classification, theory of chromatographic separation, distribution coefficient, retention, sorption, efficiency and resolution. - Column, ion exchange, paper, TLC & HPTLC chromatography etc.

**Solvent Extraction:** Distribution Coefficient, distribution ratio, percent extracted, solvent extraction of metals ions, extraction of ion association complex, extraction of metal chelates, multiple batch extraction and applications.

**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).

**Gas Chromatography:** retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

(12 Hours)

## Section – B: Physical Chemistry – 4

### Unit – 1: Quantum Chemistry & Spectroscopy

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

Postulates of quantum mechanics, quantum mechanical operators.

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

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

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

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

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

**(24 Hours)**

## **Unit – 2: Photochemistry**

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

**(6 Hours)**

## **Reference Books:**

- Skoog, D.A.; West, D.M. & Holler, F.J. *Fundamentals of Analytical Chemistry* 6<sup>th</sup> Ed., Saunders College Publishing, Fort Worth (1992).
- Dean, J. A. *Analytical Chemistry Notebook*, McGraw Hill.
- Vogel, A. I. *Vogel's Qualitative Inorganic Analysis* 7<sup>th</sup> Ed., Prentice Hall.
- Vogel, A. I. *Vogel's Quantitative Chemical Analysis* 6<sup>th</sup> Ed., Prentice Hall.
- G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).
- G. W. Castellan: *Physical Chemistry* 4th Edn. Narosa (2004).
- J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry*, Cengage Learning India Pvt. Ltd., New Delhi (2009).
- B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).
- R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
- J. D. Lee: *A New Concise Inorganic Chemistry*, E.L.B.S.
- F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
- D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
- Gary Wulfsberg: *Inorganic Chemistry*, Viva Books Pvt. Ltd.

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## **GE – E Lab: Analytical Chemistry, Quantum Chemistry & Spectroscopy**

**(60 Hours)**

### **Section – A: Inorganic Chemistry**

1. Estimation of the amount of nickel present in a given solution as bis(dimethylglyoximate) nickel(II) or aluminium as oxinate in a given solution gravimetrically.
2. Estimation of (i)  $\text{Mg}^{2+}$  or (ii)  $\text{Zn}^{2+}$  by complexometric titrations using EDTA.
3. Estimation of total hardness of a given sample of water by complexometric titration.
4. To draw calibration curve (absorbance at  $\lambda_{\text{max}}$  vs. concentration) for various concentrations of a given coloured compound and estimate the concentration of the same in a given solution.
5. Determination of the composition of the  $\text{Fe}^{3+}$  - salicylic acid complex /  $\text{Fe}^{2+}$  - phenanthroline complex in solution by Job's method.
6. Determination of concentration of  $\text{Na}^+$  and  $\text{K}^+$  using Flame Photometry.

### **Section – B: Physical Chemistry**

#### **UV/Visible spectroscopy**

- I. Study the 200-500 nm absorbance spectra of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  (in 0.1 M  $\text{H}_2\text{SO}_4$ ) and determine the  $\lambda_{\text{max}}$  values. Calculate the energies of the two transitions in different units ( $\text{J molecule}^{-1}$ ,  $\text{kJ mol}^{-1}$ ,  $\text{cm}^{-1}$ , eV).
- II. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of  $\text{K}_2\text{Cr}_2\text{O}_7$ .
- III. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

#### **Colourimetry**

- I. Verify Lambert-Beer's law and determine the concentration of  $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$  in a solution of unknown concentration
- II. Analyses the given vibration-rotation spectrum of  $\text{HCl(g)}$

#### **Reference Books:**

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

### **GE – F: Chemistry of f-Block Elements, Bio-inorganic Chemistry, Polynuclear Hydrocarbons and UV, IR Spectroscopy**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Hours**

#### **Section – A: Inorganic Chemistry – 5**

#### **Unit – 1: Chemistry of f- Block Elements**

**Chemistry of Lanthanide:** Comparative study with respect to Electronic configuration, Oxidation states, atomic and ionic radii and complex formation, Lanthanide contraction, occurrence and isolation (ion exchange and solvent extraction methods), important lanthanide compounds.

**Chemistry of Actinides:** General features and chemistry of actinides, chemistry of separation of Np, Pu and Am from U. trans-uranium elements. Similarities between the later actinides and the later lanthanides.

(10 Hours)

### Unit – 1: Radioactivity

Radioactive decay, half-life and average life of radio elements, units of radioactivity, natural radioactive disintegration series, Instrumental analysis of radioactive elements, radioactive equilibrium, group displacement law, isotope, isotone, isobars and nuclear isomerism. Application of isotope in medicine, agriculture, reaction mechanism (isotope as tracer), age of minerals, age of earth, radio carbon dating, nuclear particles, nuclear forces: meson exchange theory.

### Unit – 1: Bio-Inorganic Chemistry

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

(10 Hours)

### Section – B: Organic Chemistry – 4

#### Unit – 1: Polynuclear and heteronuclear aromatic compounds:

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

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

(10 Hours)

#### Unit – 2: Concept of Energy in Biosystems

Calorific value of food. Standard caloric content of carbohydrates, proteins and fats. Oxidation of foodstuff (organic molecules) as a source of energy for cells. Introduction to Metabolism (catabolism, anabolism), ATP: the universal currency of cellular energy, ATP hydrolysis and free energy change. Conversion of food into energy. Outline of catabolic pathways of Carbohydrate- Glycolysis, Fermentation, Krebs Cycle. Overview of catabolic pathways of Fats and Proteins. Interrelationships in the metabolic pathways of Proteins, Fats and Carbohydrates.

#### Unit – 3: Application of Spectroscopy to Simple Organic Molecules

Application of visible, ultraviolet and Infrared spectroscopy in organic molecules. Electromagnetic radiations, electronic transitions,  $\lambda_{\max}$  &  $\epsilon_{\max}$ , chromophore, auxochrome, bathochromic and hypsochromic shifts. Application of electronic spectroscopy and Woodward rules for calculating  $\lambda_{\max}$  of conjugated dienes and  $\alpha, \beta$  – unsaturated compounds.

Infrared radiation and types of molecular vibrations, functional group and fingerprint region. IR spectra of alkanes, alkenes and simple alcohols (inter and intramolecular hydrogen bonding), aldehydes, ketones, carboxylic acids and their derivatives (effect of substitution on  $>C=O$  stretching absorptions).

**(18 Hours)**

#### Reference Books:

- B. R. Puri, L. R. Sharma, and K. C. Kalia: *Principle of Inorganic Chemistry*, Milestone Publisher, New Delhi **2010**.
- W. U. Malik, G. D. Tuli, and R. D. Madan: *Selected Topic in Inorganic Chemistry*, S. Chand & Company Ltd, New Delhi, **1998**.
- I.L. Finar: *Organic Chemistry* (Vol. I & II), E.L.B.S.
- H. J. Arnikar: *Essentials of Nuclear Chemistry*.
- A. K. Das, Bioinorganic Chemistry, Books & Allied Ltd.
- John R. Dyer: *Applications of Absorption Spectroscopy of Organic Compounds*, Prentice Hall.
- R.M. Silverstein, G.C. Bassler & T.C. Morrill: *Spectroscopic Identification of Organic Compounds*, John Wiley & Sons.
- R.T. Morrison & R.N. Boyd: *Organic Chemistry*, Prentice Hall.
- Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
- Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*.
- Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Biochemistry 7<sup>th</sup> Ed.*, W. H. Freeman.
- Berg, J. M., Tymoczko, J. L. & Stryer, L. *Biochemistry 7<sup>th</sup> Ed.*, W. H. Freeman.
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#### **GE – F Lab: Chemistry of f-Block Elements, Bio-inorganic Chemistry, Polynuclear Hydrocarbons and UV, IR Spectroscopy**

**(60 Hours)**

##### **Section – A: Inorganic Chemistry**

1. Separation of mixtures by chromatography: Measure the  $R_f$  value in each case.  
(Combination of two ions to be given)

Paper chromatographic separation of  $Fe^{3+}$ ,  $Al^{3+}$  and  $Cr^{3+}$  or

Paper chromatographic separation of  $Ni^{2+}$ ,  $Co^{2+}$ ,  $Mn^{2+}$  and  $Zn^{2+}$

2. Gravimetric estimation of Cations/ Anions.

Estimation of zinc, aluminium and barium given in ore. Chloride, fluoride and sulphate in given sample.

### ***Section – B: Organic Chemistry***

1. Separation of amino acids by paper chromatography
2. Study of titration curve of glycine
3. Effect of temperature on the action of salivary amylase on starch.
4. To determine the saponification value of an oil/fat.
5. To determine the iodine value of an oil/fat
6. Differentiate between a reducing/ nonreducing sugar.
7. Extraction of DNA from onion/cauliflower
8. To synthesize aspirin by acetylation of salicylic acid and compare it with the ingredient of an aspirin tablet by TLC.

### **Reference Books:**

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

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## **GE - G: Polymer, Nuclear and Materials Chemistry**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Hours**

### ***Section – A: Polymer Chemistry***

#### **Unit – 1: Organic Polymers**

Definition of monomers and polymers. Classification of polymers. Different types of processes for polymerization and their mechanisms (ionic, free radical and Ziegler-Natta catalyst). Preparation and uses of some polymers viz., nylons, polyesters, polyvinyl chloride, Teflon, Bakelite, urea and melamineformaldehyde, resins. Natural rubber (isolation, structure and vulcanization). Synthetic elastomers – buna S, butyl rubber and polyurethane. Development of biodegradable polymers viz., polylactic acid and polyhydroxybutyric acid.

#### **Unit – 2: Inorganic and Physical Polymers**

Comparison between inorganic and organic polymers. Synthesis, structural aspects and applications of borazine, silicates and silicones.

Different schemes of classification of polymers. Molar mass of polymers. Number average and mass, average molar masses. Methods of determining molar mass by osmotic pressure and viscosity measurements.

#### **Unit – 3: Mechanisms of Polymerisation**

Types of polymers and polymerisation process, addition polymers, stereo controlled polymers, condensation polymers, radical, ionic and coordination mechanism of polymers : (i) Natural and synthetic rubber (ii) synthetic fibres, polyester, polyamides, Polyacrylates, and rayons. (iii) Plastic: Polyolefines and Polyurethanes (iv) Foaming agent plasticiser (v) Biodegradable polymers.

## ***Section – B: Nuclear and Materials Chemistry***

### **Unit – 1: Nuclear Forces, Energy and Fuels**

**Nuclear Forces:** Nuclear Radiation, forces in nucleus, nuclear stability, neutron proton ratio and binding energy, packing fraction

**Nuclear Energy:** Energy releasing fission, chain reactions, controlled release of fission energy, use of moderators, energy release in fusion reactions, principle of atomic and hydrogen bombs

**Nuclear Fuels (Uranium & Thorium):** Distribution in nature, production as nuclear fuels, enrichment of uranium, extraction of thorium and uranium from their ores.

### **Unit – 2: Extraction of Metals and Non-Metals**

Techniques and application of extraction of elements from their important ores – bauxite, lime stones other ores of the region.

### **Unit – 3: Chemistry of Nano-Materials**

Nanoscience – principles, structure determination, Synthesis, photo-physical properties and applications of nano particles consisting of gold, silver and iron.

### **Recommended Texts:**

- Principles of Polymer Chemistry, Ravve, A. 2nd ed.,
- Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3<sup>rd</sup> ed. Oxford University Press (2005)
- Seymour/ Carraher's Polymer Chemistry, 9<sup>th</sup> ed. by Charles E. Carraher, Jr. (2013).
- Petr Munk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2<sup>nd</sup> ed. John Wiley & Sons (2002)
- Joel R. Fried, Polymer Science and Technology, 2<sup>nd</sup> ed. Prentice-Hall (2003)
- Essentials of Nuclear Chemistry by H. J. Arnikar
- Chemistry of Materials by Rao

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## **GE – G Lab: Polymer, Nuclear and Materials Chemistry**

**(60 Hours)**

### ***Section – A: Polymer Chemistry***

#### 4. Polymer synthesis

- (ix) Free radical solution polymerization of styrene (St)/Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).
  - (c) Purification of monomer
  - (d) Polymerization using benzoyl peroxide (BPO)/2,2'-azo-bis-isobutyl-nitrile (AIBN)
- (x) Preparation of nylon 66/6
- (xi) Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein
  - (d) Preparation of IPC
  - (e) Purification of IPC
  - (f) Interfacial polymerization
- (xii) Redox polymerization of acrylamide
- (xiii) Precipitation polymerization of acrylonitrile
- (xiv) Preparation of urea-formaldehyde resin
- (xv) Preparations of novalac resin/resold resin
- (xvi) Microscale Emulsion Polymerization of Poly(methylacrylate)

#### *Section – B: Materials Chemistry*

- Verification of the Beer-Lambert law using gold/silver nanoparticles.
- Metal based nanoparticles are examined by converting *p*-nitrophenol to *p*-aminophenol.
- Synthesis and characterization of mixed metal oxide (bimetallic and oxides)
- Preparation and characterization of nanomaterials by wet chemical routes (sol-gel, reverse micelles, hydrothermal, co-precipitation, *etc.*)

#### **Recommended Texts:**

- Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3<sup>rd</sup> ed. Oxford University Press (2005)
- Seymour/ Carraher's Polymer Chemistry, 9<sup>th</sup> ed. by Charles E. Carraher, Jr. (2013).
- Petr Munk and Tejjraj M. Aminabhavi, Introduction to Macromolecular Science, 2<sup>nd</sup> ed. John Wiley & Sons (2002)
- Joel R. Fried, Polymer Science and Technology, 2<sup>nd</sup> ed. Prentice-Hall (2003)
- Furniss, B.S.; Hannaford, A.J.; Rogers, V.; Smith, P.W.G.; Tatchell, A.R. *Vogel's Textbook of Practical Organic Chemistry*, ELBS.
- Pradeep, T. *A Textbook of Nanoscience and Nanotechnology*, McGraw Hill Edu. New Delhi, (2015).