



# UNIVERSITY OF CALCUTTA

**GURUPADA SAREN**

**SECRETARY**

COUNCILS FOR UNDERGRADUATE STUDIES,  
UNIVERSITY OF CALCUTTA.

Ref.No : CUS/ 56 /18  
Dated the 01<sup>st</sup> February, 2018

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To  
The Principals/T.I.C.  
of all the Undergraduate Colleges  
offering B.Sc. (Honours) in Chemistry  
affiliated to the University of Calcutta

Sir/Madam,

The undersigned is to inform you that the proposed **revised semesterised draft Syllabus for Chemistry (Honours) Courses of Studies under CBCS has been uploaded in the Calcutta University website ([www.caluniv.ac.in](http://www.caluniv.ac.in)).**

The said syllabus has been prepared by the **U.G. Board of Studies in Chemistry, C.U.**, suppose to be implemented from the academic session 2018-2019

You are requested kindly to go through it and send your feedback within 15<sup>th</sup> February, 2018.

In this regard you may send your observation/ suggestion to the **Department of U.G. Councils, C.U.** or through email ([u.g.councilsc.u@gmail.com](mailto:u.g.councilsc.u@gmail.com)), and you also may contact **Prof. Chaitali Mukhopadhyay**, Department of Chemistry, C.U. through e-mail ([cmchem@caluniv.ac.in](mailto:cmchem@caluniv.ac.in) ).

Your cooperation in this regard will be highly appreciated. Kindly treat the matter as urgent.

Thanking you,

Yours faithfully,

  
Secretary

# **MODEL COURSE CURRICULUM UNDER CHOICE BASED CREDIT SYSTEM**

**PROPOSED DRAFT SYLLABUS  
FOR**

**BACHELOR  
IN CHEMISTRY (HONOURS)**



**UNIVERSITY OF CALCUTTA**

# 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</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	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	4×2=8	4×1=4
<b>(4 Papers)</b>		
<ul style="list-style-type: none"> <li>• <b>Optional Dissertation or project work in place of one Discipline Specific Elective paper (6 credits) in 6<sup>th</sup> Semester</b></li> </ul>		
<b>III. Ability Enhancement Courses</b>		
<b>1. Ability Enhancement Compulsory</b>		
<b>(2 Papers of 2 credit each)</b>	2×2=4	2×2=4
Environmental Science		
English/MIL Communication		
<b>2. Ability Enhancement Elective (Skill Based)</b>		
(Minimum 2)	2×2=4	2×2=4
<b>(2 Papers of 2 credit each)</b>		
<b>Total credit</b>	<b>140</b>	<b>140</b>

**Institute should evolve a system/policy about ECA/ General Interest/Hobby/Sports/NCC/NSS/related courses on its own.**

**PROPOSED SCHEME FOR CHOICE BASED CREDIT SYSTEM IN**  
**B. SC. HONOURS (CHEMISTRY)**

SEM	Core Course (14)	Ability Enhancement Compulsory Course (AECC) ( 2)	Ability Enhancement Compulsory Course (AECC) ( 2) (Skill Based)	Elective: Discipline Specific (DSE) (4)	Elective: Generic (4) (for Major) (6) (for minor)
I	Organic-I (Core Course-I)				GE-1
	Inorganic-I (Core Course-II)				Inorganic-I
					Physical -I
II	Physical -I (Core Course-III)				GE-2
	Organic-II (Core Course-IV)				Organic-I
					Analytical & Environment
III	Physical-II (Core Course-V)				GE-3
	Inorganic-II (Core Course-VI)				Inorganic-II
	Organic-III (Core Course-VII)				Physical-II
IV	Physical-III (Core Course-VIII)				GE-4
	Inorganic-III (Core Course-IX)				Organic-II
	Organic-IV (Core Course-X)				Analytical & Industrial-I
V	Physical- IV (Core Course-XI)			DSE-1	GE-5(for Chemistry Minor)

	Organic-V (Core Course- XII)			DSE-2	Inorganic-III Physical-III
VI	Inorganic-IV (Core Course- XIII)			DSE-3	GE-6 (for Chemistry Minor)
	Physical-V (Core Course- XIV)			DSE-4	Organic-III Analytical & Industrial-II

### Important recommendations

- **DSE-I Advanced Inorganic Chemistry is compulsory**(This recommendation is to maintain equal importance of all three major sections of Chemistry)
- **From DSE-2 to DSE-7 students are free to choose any Three (3) courses.**
- All graphs for Physical / Inorganic /Analytical Chemistry Courses must be done using Microsoft Excel.
- Each college should take necessary measures to ensure they should have the following facilities:
  1. UV-VIS Spectrophotometer with printer.
  2. FT-IR spectrophotometer with printer.
  3. Internet facility.
  4. Requisite number of computers (One computer for 3-4 students).

**For proper maintenance of above mentioned facilities, clean & dry AC rooms are mandatory.**

<b>SEMESTER</b>	<b>COURSE OPTED</b>	<b>COURSE NAME</b>	<b>Credits</b>
<b>I</b>	<b>Ability Enhancement Compulsory Course –I</b>	<b>English Communications/ Environmental Science</b>	<b>2</b>
	<b>Core Course-I</b>	<b>Organic Chemistry-I</b>	<b>4</b>
	<b>Core Course-I Practical</b>	<b>Organic Chemistry-I Lab</b>	<b>2</b>
	<b>Core Course-II</b>	<b>Inorganic Chemistry -I</b>	<b>4</b>
	<b>Core Course-II Practical</b>	<b>Inorganic Chemistry -I Lab</b>	<b>2</b>
	<b>Generic Elective -1</b>	<b>GE-1</b>	<b>4</b>
	<b>Generic Elective -1 Practical</b>		<b>2</b>
<b>II</b>	<b>Ability Enhancement Compulsory Course-II</b>	<b>English Communications/ Environmental Science</b>	<b>2</b>
	<b>Core Course-III</b>	<b>Physical Chemistry -I</b>	<b>4</b>
	<b>Core Course-III Practical</b>	<b>Physical Chemistry -I Lab</b>	<b>2</b>
	<b>Core Course-IV</b>	<b>Organic Chemistry-II</b>	<b>4</b>
	<b>Core Course-IV Practical</b>	<b>Organic Chemistry-II Lab</b>	<b>2</b>
	<b>Generic Elective -2</b>	<b>GE-2</b>	<b>4</b>
	<b>Generic Elective -2 Practical</b>		<b>2</b>
<b>III</b>	<b>Core Course-V</b>	<b>Physical Chemistry-II</b>	<b>4</b>
	<b>Core Course-V Practical</b>	<b>Physical Chemistry-II Lab</b>	<b>2</b>
	<b>Core Course-VI</b>	<b>Inorganic Chemistry-II</b>	<b>4</b>
	<b>Core Course-VI Practical</b>	<b>Inorganic Chemistry-II Lab</b>	<b>2</b>
	<b>Core Course-VII</b>	<b>Organic Chemistry-III</b>	<b>4</b>
	<b>Core Course-VII Practical</b>	<b>Organic Chemistry-III Lab</b>	<b>2</b>
	<b>Skill Enhancement Course 1 (T1)</b>	<b>SEC-1</b>	<b>2</b>
	<b>Generic Elective -3</b>	<b>GE-3</b>	<b>4</b>
	<b>Generic Elective -3 Practical</b>		<b>2</b>
<b>IV</b>	<b>Core Course-VIII</b>	<b>Physical Chemistry-III</b>	<b>4</b>
	<b>Course-VIII Practical</b>	<b>Physical Chemistry-III Lab</b>	<b>2</b>
	<b>Core Course-IX</b>	<b>Inorganic Chemistry-III</b>	<b>4</b>
	<b>Course-IX Practical</b>	<b>Inorganic Chemistry-III Lab</b>	<b>2</b>
	<b>Core Course-X</b>	<b>Organic Chemistry-IV</b>	<b>4</b>
	<b>Course-X Practical</b>	<b>Organic Chemistry-IV Lab</b>	<b>2</b>
	<b>Skill Enhancement Course -2 (T2 OR T3)</b>	<b>SEC -2</b>	<b>2</b>
	<b>Generic Elective -4</b>	<b>GE-4</b>	<b>4</b>
	<b>Generic Elective -4 Practical</b>		<b>2</b>
<b>V</b>	<b>Core Course-XI</b>	<b>Physical Chemistry -IV</b>	<b>4</b>
	<b>Core Course-XI Practical</b>	<b>Physical Chemistry -IV Lab</b>	<b>2</b>
	<b>Core Course-XII</b>	<b>Organic Chemistry-V</b>	<b>4</b>
	<b>Core Course-XII Practical</b>	<b>Organic Chemistry-V Lab</b>	<b>2</b>

	<b>Discipline Specific Elective -1</b>	<b>DSE-1</b>	<b>4</b>
	<b>Discipline Specific Elective -1 Practical</b>	<b>DSE-1 Lab</b>	<b>2</b>
	<b>Discipline Specific Elective -2</b>	<b>DSE-2</b>	<b>4</b>
	<b>Discipline Specific Elective -2 Practical</b>	<b>DSE-2 Lab</b>	<b>2</b>
<b>VI</b>	<b>Core Course-XIII</b>	<b>Inorganic Chemistry-IV</b>	<b>4</b>
	<b>Core Course-XIII Practical</b>	<b>Inorganic Chemistry-IV Lab</b>	<b>2</b>
	<b>Core Course-XIV</b>	<b>Physical Chemistry-V</b>	<b>4</b>
	<b>Core Course-XIV Practical</b>	<b>Physical Chemistry-V Lab</b>	<b>2</b>
	<b>Discipline Specific Elective -3</b>	<b>DSE-3</b>	<b>4</b>
	<b>Discipline Specific Elective -3 Practical</b>	<b>DSE-3 Lab</b>	<b>2</b>
	<b>Discipline Specific Elective-4</b>	<b>DSE-4</b>	<b>4</b>
	<b>Discipline Specific Elective-4 Practical</b>	<b>DSE-4 Lab</b>	<b>2</b>
<b>Total Credits</b>			<b>140</b>

**Core Papers (C): (Credit: 06 each)**

1. Organic Chemistry I: (4 + 4)
2. Inorganic Chemistry I: (4 + 4)
3. : Physical Chemistry I (4 + 4)
4. Organic Chemistry II: (4 + 4)
5. Physical Chemistry II: (4 + 4)
6. Inorganic Chemistry II: (4 + 4)
7. Organic Chemistry III: (4 + 4)
8. Physical Chemistry III: (4 + 4)
9. Inorganic Chemistry III: (4 + 4)
10. Organic Chemistry IV: (4 + 4)
11. Physical Chemistry IV: (4 + 4)
12. Organic Chemistry V: (4 + 4)
13. Inorganic Chemistry IV: (4 + 4)
14. Physical Chemistry V: (4 + 4)

**Discipline Specific Electives: (Credit: 06 each) (3 courses to be selected from DSE 2-7)**

1. Advanced Inorganic Chemistry(4) + Lab (4) --- **COMPULSORY**
2. Analytical Methods in Chemistry (4) + Lab (4)
3. Application of Computers in Chemistry (4) + Lab (4)
4. Green Chemistry (4) + Lab (4)
5. Inorganic Materials of Industrial Importance (4) + Lab (4)
6. Polymer Chemistry (4) + Lab (4)
7. Molecular Modelling and Drug Design(4) + Lab (4)

✓ The numbers in the parenthesis represent the number of lectures per week.

✓ Each lecture is of 1 hr duration for both theory and practical classes.

# **CORE COURSE (HONOURS) IN CHEMISTRY**

## **SEMESTER-I**

### **CHEMISTRY -C I: ORGANIC CHEMISTRY-I**

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

**Theory: 60 Lectures**

**Basics of Organic Chemistry**

**Bonding and Physical Properties**

**(20 Lectures)**

*Valence Bond Theory:* concept of hybridisation, shapes of molecules, resonance (including hyperconjugation); calculation of formal charges and double bond equivalent (DBE); orbital pictures of bonding ( $sp^3$ ,  $sp^2$ ,  $sp$ : C-C, C-N & C-O systems and *s-cis* and *s-trans* geometry for suitable cases).

*Electronic displacements:* inductive effect, field effect, mesomeric effect, resonance energy; bond polarization and bond polarizability; electromeric effect; steric effect, steric inhibition of resonance.

*MO theory:* qualitative idea about molecular orbitals, bonding and antibonding interactions, idea about  $\sigma$ ,  $\sigma^*$ ,  $\pi$ ,  $\pi^*$ ,  $n$  – MOs; basic idea about Frontier MOs (FMO); concept of HOMO, LUMO and SOMO; interpretation of chemical reactivity in terms of FMO interactions; sketch and energy levels of  $\pi$  MOs of i) acyclic p orbital system (C=C, conjugated diene, triene, allyl and pentadienyl systems) ii) cyclic p orbital system (neutral systems: [4], [6]-annulenes; charged systems: 3-,4-,5-membered ring systems); Hückel's rules for aromaticity up to [10]-annulene (including mononuclear heterocyclic compounds up to 6-membered ring); concept of antiaromaticity and homoaromaticity; non-aromatic molecules; Frost diagram; elementary idea about  $\alpha$  and  $\beta$ ; measurement of delocalization energies in terms of  $\beta$  for buta-1,3-diene, cyclobutadiene, hexa-1,3,5-triene and benzene.

*Physical properties:* influence of hybridization on bond properties: bond dissociation energy (BDE) and bond energy; bond distances, bond angles; concept of bond angle strain (Baeyer's strain theory); melting point/boiling point and solubility of common organic compounds in terms of covalent & non-covalent intermolecular forces; polarity of molecules and dipole moments; relative stabilities of isomeric hydrocarbons in terms of heat of hydrogenation, heat of combustion and heat of formation.

**General Treatment of Reaction Mechanism I**

**(10 Lectures)**

*Mechanistic classification:* ionic, radical and pericyclic (definition and example);



reaction type: addition, elimination and substitution reactions (definition and example); nature of bond cleavage and bond formation: homolytic and heterolytic bond fission, homogenic and heterogenic bond formation; curly arrow rules in representation of mechanistic steps; reagent type: electrophiles and nucleophiles (elementary idea); electrophilicity and nucleophilicity in terms of FMO approach.

*Reactive intermediates:* carbocations (carbenium and carbonium ions), carbanions, carbon radicals, carbenes: generation and stability, structure using orbital picture and electrophilic/nucleophilic behavior of reactive intermediates (elementary idea).

## **Stereochemistry I**

**(30 Lectures)**

*Bonding geometries of carbon compounds and representation of molecules:* tetrahedral nature of carbon and concept of asymmetry; Fischer, sawhorse, flying-wedge and Newman projection formulae and their inter translations.

*Concept of chirality and symmetry:* symmetry elements and point groups ( $C_{av}$ ,  $C_{nh}$ ,  $C_{nv}$ ,  $C_n$ ,  $D_{ch}$ ,  $D_{nh}$ ,  $D_{nd}$ ,  $D_n$ ,  $S_n$  ( $C_s$ ,  $C_i$ ); molecular chirality and centre of chirality; asymmetric and dissymmetric molecules; enantiomers and diastereomers; concept of epimers; concept of stereogenicity, chirotopicity and pseudoasymmetry; chiral centres and number of stereoisomerism: systems involving 1/2/3-chiral centre(s) (AA, AB, ABA and ABC types).

*Relative and absolute configuration:* D/L and R/S descriptors; erythro/threo and meso nomenclature of compounds; syn/anti nomenclatures for aldols; E/Z descriptors for C=C, conjugated diene, triene, C=N and N=N systems; combination of R/S- and E/Z-isomerisms.

*Optical activity of chiral compounds:* optical rotation, specific rotation and molar rotation; racemic compounds, racemisation (through cationic, anionic, radical intermediates and through reversible formation of stable achiral intermediates); resolution of acids, bases and alcohols via diastereomeric salt formation; optical purity and enantiomeric excess; invertomerism of chiral trialkylamines.

*Chirality arising out of stereoaxis:* stereoisomerism of substituted cumulenes with even and odd number of double bonds; chiral axis in allenes, alkylidenecycloalkanes and biphenyls; atropisomerism.

*Concept of prostereoisomerism:* prostereogenic centre; concept of (pro)<sup>n</sup>-chirality: topicity of ligands and faces (elementary idea); pro-R/pro-S, pro-E/pro-Z and Re/Si descriptors; pro-r and pro-s descriptors of ligands on propseudoasymmetric centre.

### **Reference Books**

1. Clayden, J., Greeves, N. & Warren, S. *Organic Chemistry*, Second edition, Oxford University Press, 2012.
2. Keeler, J., Wothers, P. *Chemical Structure and Reactivity – An Integrated approach*, Oxford University Press.

3. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
  4. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
  5. Carey, F. A., Giuliano, R. M. *Organic Chemistry*, Eighth edition, McGraw Hill Education, 2012.
  6. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London, 1994.
  7. Nasipuri, D. *Stereochemistry of Organic Compounds*, Wiley Eastern Limited.
  8. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
  9. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education)
  10. Fleming, I. *Molecular Orbitals and Organic Chemical Reactions*, Reference/Student Edition, Wiley, 2009.
  11. James, J., Peach, J. M. *Stereochemistry at a Glance*, Blackwell Publishing, 2003.
  12. Robinson, M. J. T., *Stereochemistry*, Oxford Chemistry Primer, Oxford University Press, 2005.
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## **CHEMISTRY LAB-C I LAB**

**(60 Lectures)**

**1. Separation** based upon solubility, by using common laboratory reagents like water (cold, hot), dil. HCl, dil. NaOH, dil. NaHCO<sub>3</sub>, etc., of components of a binary solid mixture; purification of **any one** of the separated components by crystallization and determination of its melting point. The composition of the mixture may be of the following types [**ANY THREE**]: *p*-Nitrobenzoic acid/*p*-Aminobenzoic acid; *p*-Nitrotoluene/*p*-Anisidine; benzoic acid/ naphthalene; urea/phenyl-benzoate; *p*-toluidine/benzophenone; *p*-chlorobenzoic acid/ benzophenone; etc. USE of pH PAPER is recommended.

**2. Determination of boiling point** of common organic liquid compounds [ANY FIVE] e.g., ethanol, cyclohexane, chloroform, ethyl methyl ketone, cyclohexanone, acetylacetone, anisole, crotonaldehyde, mesityl oxide, etc. [Boiling point of the chosen organic compounds should preferably be less than 160 °C]

### **3. Identification of a Pure Organic Compound**

*Solid compounds*: oxalic acid, tartaric acid, citric acid, succinic acid, resorcinol, urea, glucose, cane sugar, benzoic acid and salicylic acid

*Liquid Compounds*: formic acid, acetic acid, methyl alcohol, ethyl alcohol, acetone, aniline, dimethylaniline, benzaldehyde, chloroform and nitrobenzene

### **Reference Books**

1. Bhattacharyya, R. C, *A Manual of Practical Chemistry*.
  2. Vogel, A. I. *Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis*, CBS Publishers and Distributors.
  3. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009).
  4. Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012).
  5. Dutta, S, B. *Sc. Honours Practical Chemistry*, Bharati Book Stall.
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## **CHEMISTRY -C II: INORGANIC CHEMISTRY-I**

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

**Theory: 60 Lectures**

### **Extra nuclear Structure of atom**

**(14 Lectures)**

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. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s*, *p*, *d* and *f* orbitals. Pauli's Exclusion Principle, Hund's rules and multiplicity, Exchange energy, Aufbau principle and its limitations, Ground state Term symbols of atoms and ions for atomic number upto 30.

### **Chemical periodicity**

**(10 Lectures)**

Modern IUPAC Periodic table, Effective nuclear charge, screening effects and penetration, Slater's rules, atomic radii, ionic radii (Pauling's univalent), covalent radii, lanthanide contraction. Ionization potential, electron affinity and electronegativity (Pauling's, Mulliken's and Allred-Rochow's scales) and factors influencing these properties, group electronegativities. Group trends and periodic trends in these properties in respect of s-, p- and d-block elements. Secondary periodicity, Relativistic Effect, Inert pair effect.

### **Radioactivity**

**(10 Lectures)**

Nuclear stability and nuclear binding energy. Nuclear forces: meson exchange theory. Nuclear models (elementary idea): Concept of nuclear quantum number, magic numbers. Nuclear Reactions: Artificial radioactivity, transmutation of elements, fission, fusion and spallation. Nuclear energy and power generation. Separation and uses of isotopes. Radio chemical methods: principles of determination of age of rocks and minerals, radio carbon dating, hazards of radiation and safety measures.

**Acid-Base reactions****(12 Lectures)**

Acid-Base concept: Arrhenius concept, theory of solvent system (in H<sub>2</sub>O, NH<sub>3</sub>, SO<sub>2</sub> and HF), Bronsted-Lowry's concept, relative strength of acids, Pauling's rules. Lux-Flood concept, Lewis concept, group characteristics of Lewis acids, solvent levelling and differentiating effects. Thermodynamic acidity parameters, Drago-Wayland equation. Superacids, Gas phase acidity and proton affinity; HSAB principle. Acid-base equilibria in aqueous solution (Proton transfer equilibria in water), pH, buffer. Acid-base neutralisation curves; indicator, choice of indicators.

**Redox Reactions and precipitation reactions****(14 Lectures)**

Ion-electron method of balancing equation of redox reaction. Elementary idea on standard redox potentials with sign conventions, Nernst equation (without derivation). Influence of complex formation, precipitation and change of pH on redox potentials; formal potential. Feasibility of a redox titration, redox potential at the equivalence point, redox indicators. Redox potential diagram (Latimer and Frost diagrams) of common elements and their applications. Disproportionation and comproportionation reactions (typical examples). Solubility product principle, common ion effect and their applications to the precipitation and separation of common metallic ions as hydroxides, sulfides, phosphates, carbonates, sulfates and halides.

**Reference Books**

1. Lee, J. D. *Concise Inorganic Chemistry*, 5<sup>th</sup> Ed., Wiley India Pvt. Ltd., 2008.
2. Douglas, B.E. and McDaniel, D.H. *Concepts & Models of Inorganic Chemistry* Oxford, 1970.
3. Day, M.C. and Selbin, J. *Theoretical Inorganic Chemistry*, ACS Publications, 1962.
4. Atkin, P. *Shriver & Atkins' Inorganic Chemistry*, 5<sup>th</sup> Ed., Oxford University Press (2010).
5. Cotton, F.A., Wilkinson, G. and Gaus, P.L., *Basic Inorganic Chemistry* 3<sup>rd</sup> Ed.; Wiley India.
6. Sharpe, A.G., *Inorganic Chemistry*, 4<sup>th</sup> Indian Reprint (Pearson Education) 2005.
7. 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.
8. Atkins, P.W. & Paula, J. *Physical Chemistry*, Oxford Press, 2006.
9. Mingos, D.M.P., *Essential trends in inorganic chemistry*. Oxford University Press (1998).
10. Winter, M. J., The Orbitron, <http://winter.group.shef.ac.uk/orbitron/> (2002). An illustrated gallery of atomic and molecular orbitals.
11. Burgess, J., *Ions in solution: basic principles of chemical interactions*. Ellis Horwood (1999).

## **CHEMISTRY LAB-C II LAB**

### **60 Lectures**

#### **Acid and Base Titrations:**

1. Estimation of carbonate and hydroxide present together in mixture
2. Estimation of carbonate and bicarbonate present together in a mixture.
3. Estimation of free alkali present in different soaps/detergents.

#### **Oxidation-Reduction Titrations:**

1. Estimation of Fe(II) using standardized  $\text{KMnO}_4$  solution
2. Estimation of oxalic acid and sodium oxalate in a given mixture
3. Estimation of Fe(II) and Fe(III) in a given mixture using  $\text{K}_2\text{Cr}_2\text{O}_7$  solution.
4. Estimation of Fe(III) and Mn(II) in a mixture using standardized  $\text{KMnO}_4$  solution
5. Estimation of Fe(III) and Cu(II) in a mixture using  $\text{K}_2\text{Cr}_2\text{O}_7$ .
6. Estimation of Fe(III) and Cr(III) in a mixture using  $\text{K}_2\text{Cr}_2\text{O}_7$ .

#### **Reference Books**

1. Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis* 6th Ed., Pearson, 2009.
  2. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015
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## SEMESTER-II

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### **CHEMISTRY -C III: PHYSICAL CHEMISTRY-I**

(Credits: Theory-04, Practicals-02)

**Theory: 60 Lectures**

#### **Kinetic Theory and Gaseous state (15 Lectures)**

Kinetic Theory of gases: Concept of pressure and temperature; Collision of gas molecules; Collision diameter; Collision number and mean free path; Frequency of binary collisions (similar and different molecules); Wall collision and rate of effusion

Maxwell's distribution of speed and energy: Nature of distribution of velocities, Maxwell's distribution of speeds in one, two and three dimensions; Kinetic energy distribution in one, two and three dimensions, calculations of average, root mean square and most probable values in each case; Calculation of number of molecules having energy  $\geq \epsilon$ , Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases

Real gas and virial equation: Deviation of gases from ideal behavior; compressibility factor; Boyle temperature; Andrew's and Amagat's plots; van der Waals equation and its features; its derivation and application in explaining real gas behaviour, other equations of state (Berthelot, Dietrici); Existence of critical state, Critical constants in terms of van der Waals constants; Law of corresponding states; virial equation of state; van der Waals equation expressed in virial form and significance of second virial coefficient; Intermolecular forces (Debye, Keesom and London interactions; Lennard-Jones potential - elementary idea)

#### **Chemical Thermodynamics I (12 Lectures)**

Zeroth and 1<sup>st</sup> law of Thermodynamics: Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics; Concept of heat, work, internal energy and statement of first law; enthalpy,  $H$ ; relation between heat capacities, calculations of  $q$ ,  $w$ ,  $\Delta U$  and  $\Delta H$  for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions; Joule's experiment and its consequence

Thermochemistry: Standard states; Heats of reaction; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; Laws of thermochemistry; bond energy, bond dissociation energy and resonance energy from thermochemical data, Kirchhoff's equations and effect of pressure on enthalpy of reactions; Adiabatic flame temperature; explosion temperature

#### **Transport processes (06 Lectures)**

Fick's law: Flux, force, phenomenological coefficients & their inter-relationship (general form), different examples of transport properties

Viscosity: General features of fluid flow (streamline flow and turbulent flow); Newton's equation, viscosity coefficient; Poiseuille's equation; principle of

determination of viscosity coefficient of liquids by falling sphere method; Temperature variation of viscosity of liquids and comparison with that of gases

**Ionic equilibrium:**

**(12 Lectures)**

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

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

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

Multistage equilibrium in polyelectrolyte systems; hydrolysis and hydrolysis constants.

**Chemical kinetics**

**(15 Lectures)**

Rate law, order and molecularity: Introduction of rate law, Extent of reaction; rate constants, order; Forms of rates of First, second and nth order reactions; Pseudo first order reactions (example using acid catalyzed hydrolysis of methyl acetate); Determination of order of a reaction by half-life and differential method; Opposing reactions, consecutive reactions and parallel reactions (with explanation of kinetic and thermodynamic control of products; all steps first order)

Role of Temperature and theories of reaction rate: Temperature dependence of rate constant; Arrhenius equation, energy of activation; Rate-determining step and steady-state approximation – explanation with suitable examples; Collision theory; Lindemann theory of unimolecular reaction; outline of Transition State theory (classical treatment)

Homogeneous catalysis: Homogeneous catalysis with reference to acid-base catalysis; Enzyme catalysis; Michaelis-Menten equation, Lineweaver-Burk plot, turn-over number.

**Reference Books**

1. Atkins, P. W. & Paula, J. de *Atkins' Physical Chemistry*, Oxford University Press
2. Castellan, G. W. *Physical Chemistry*, Narosa
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
5. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill
6. Maron, S. & Prutton *Physical Chemistry*
7. Ball, D. W. *Physical Chemistry*, Thomson Press
8. Mortimer, R. G. *Physical Chemistry*, Elsevier
9. Laidler, K. J. *Chemical Kinetics*, Pearson
10. Glasstone, S. & Lewis, G.N. *Elements of Physical Chemistry*

11. Rakshit, P.C., *Physical Chemistry* Sarat Book House
  12. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill
  13. Klotz, I.M., Rosenberg, R. M. *Chemical Thermodynamics: Basic Concepts and Methods* Wiley
  14. Kapoor K.L, A Text Book Of Physical Chemistry ,McGrawHill, Volume I,II,V
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## **CHEMISTRY LAB-C III LAB**

**(60 Lectures)**

Experiment 1: Determination of pH of unknown solution (buffer), by color matching method

Experiment 2: Determination of heat of neutralization of a strong acid by a strong base

Experiment 3: Study of kinetics of acid-catalyzed hydrolysis of methyl acetate

Experiment 4: Study of kinetics of decomposition of  $\text{H}_2\text{O}_2$

Experiment 5: Study of viscosity of unknown liquid (glycerol, sugar) with respect to water.

Experiment 6: Determination of solubility of sparingly soluble salt in water, in electrolyte with common ions and in neutral electrolyte (using common indicator)

### **Reference Books**

1. Viswanathan, B., Raghavan, P.S. *Practical Physical Chemistry* Viva Books (2009)
  2. Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis* 6th Ed., Pearson
  3. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007)
  4. Palit, S.R., De, S. K. *Practical Physical Chemistry* Science Book Agency
  5. Levitt, B. P. edited *Findlay's Practical Physical Chemistry* Longman Group Ltd.
  6. Gurtu, J. N., Kapoor, R., *Advanced Experimental Chemistry* S. Chand & Co. Ltd.
  7. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015
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## **CHEMISTRY -C IV: ORGANIC CHEMISTRY-II**

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

**Theory: 60 Lectures**

### **Stereochemistry II**

**(10 Lectures)**

*Conformation:* conformational nomenclature: eclipsed, staggered, *gauche*, *syn* and *anti*; dihedral angle, torsion angle; Klyne-Prelog terminology; *P/M* descriptors; energy barrier of rotation, concept of torsional and steric strains; relative stability of conformers on the basis of steric effect, dipole-dipole interaction and H-bonding; *butane gauche* interaction; conformational analysis of ethane, propane, *n*-butane, 2-methylbutane and 2,3-dimethylbutane; haloalkane, 1,2-dihaloalkanes and 1,2-diols (up to four carbons); 1,2-halohydrin; conformation of conjugated systems (*s-cis* and *s-trans*).

### **General Treatment of Reaction Mechanism II**

**(20 Lectures)**

*Reaction thermodynamics:* free energy and equilibrium, enthalpy and entropy factor, calculation of enthalpy change via BDE, intermolecular & intramolecular reactions.

*Concept of organic acids and bases:* effect of structure, substituent and solvent on acidity and basicity; proton sponge; gas-phase acidity and basicity; comparison between nucleophilicity and basicity; HSAB principle; application of thermodynamic principles in acid-base equilibria.

*Tautomerism:* prototropy (keto-enol, nitro - *aci*-nitro, nitroso-oximino, diazo-amino and enamine-imine systems); valence tautomerism and ring-chain tautomerism; composition of the equilibrium in different systems (simple carbonyl; 1,2- and 1,3-dicarbonyl systems, phenols and related systems), factors affecting keto-enol tautomerism; application of thermodynamic principles in tautomeric equilibria.

*Reaction kinetics:* rate constant and free energy of activation; concept of order and molecularity; free energy profiles for one-step, two-step and three-step reactions; catalyzed reactions: electrophilic and nucleophilic catalysis; kinetic control and thermodynamic control of reactions; isotope effect: primary and secondary kinetic isotopic effect ( $k_H/k_D$ ); principle of microscopic reversibility; Hammond's postulate.

### **Substitution and Elimination Reactions**

**(15 Lectures)**

*Free-radical substitution reaction:* halogenation of alkanes, mechanism (with evidence) and stereochemical features; reactivity-selectivity principle in the light of Hammond's postulate.

*Nucleophilic substitution reactions:* substitution at  $sp^3$  centre: mechanisms (with evidence), relative rates & stereochemical features:  $S_N1$ ,  $S_N2$ ,  $S_N2'$ ,  $S_N1'$  (allylic rearrangement) and  $S_{Ni}$ ; effects of solvent, substrate structure, leaving group and nucleophiles (including ambident nucleophiles, cyanide & nitrite); substitutions

involving NGP; role of crown ethers and phase transfer catalysts; [systems: alkyl halides, allyl halides, benzyl halides, alcohols, ethers, epoxides].

*Elimination reactions:* E1, E2, E1cB and Ei (pyrolytic *syn* eliminations); formation of alkenes and alkynes; mechanisms (with evidence), reactivity, regioselectivity (Saytzeff/Hofmann) and stereoselectivity; comparison between substitution and elimination; importance of Bredt's rule relating to the formation of C=C.

## **Chemistry of alkenes and alkynes**

**(15 Lectures)**

*Addition to C=C:* mechanism (with evidence wherever applicable), reactivity, regioselectivity (Markownikoff and anti-Markownikoff additions) and stereoselectivity; reactions: hydrogenation, halogenations, iodolactonisation, hydrohalogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, epoxidation, *syn* and *anti*-hydroxylation, ozonolysis, addition of singlet and triplet carbenes; electrophilic addition to diene (conjugated dienes and allene); radical addition: HBr addition; mechanism of allylic and benzylic bromination in competition with brominations across C=C; use of NBS; Birch reduction of benzenoid aromatics; interconversion of *E* - and *Z* - alkenes; contra-thermodynamic isomerization of internal alkenes.

*Addition to C≡C (in comparison to C=C):* mechanism, reactivity, regioselectivity (Markownikoff and anti-Markownikoff addition) and stereoselectivity; reactions: hydrogenation, halogenations, hydrohalogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, dissolving metal reduction of alkynes (Birch); reactions of terminal alkynes by exploring its acidity; interconversion of terminal and non-terminal alkynes.

### **Reference Books**

1. Clayden, J., Greeves, N., Warren, S. *Organic Chemistry*, Second edition, Oxford University Press 2012.
2. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
3. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
4. Carey, F. A. & Giuliano, R. M. *Organic Chemistry*, Eighth edition, McGraw Hill Education, 2012.
5. Loudon, G. M. *Organic Chemistry*, Fourth edition, Oxford University Press, 2008.
6. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London, 1994.
7. Nasipuri, D. *Stereochemistry of Organic Compounds*, Wiley Eastern Limited.
8. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
9. Finar, I. L. *Organic Chemistry (Volume 1)* Pearson Education.
10. Graham Solomons, T.W., Fryhle, C. B. *Organic Chemistry*, John Wiley & Sons, Inc.

11. James, J., Peach, J. M. *Stereochemistry at a Glance*, Blackwell Publishing, 2003.
12. Robinson, M. J. T., *Stereochemistry*, Oxford Chemistry Primer, Oxford University Press, 2005.
13. Maskill, H., *Mechanisms of Organic Reactions*, Oxford Chemistry Primer, Oxford University Press.

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## **CHEMISTRY LAB-C IV LAB**

### **60 Lectures**

#### **Organic Preparations**

A. The following reactions are to be performed, noting the yield of the crude product:

1. Nitration of aromatic compounds
2. Condensation reactions
3. Hydrolysis of amides/imides/esters
4. Acetylation of phenols/aromatic amines
5. Benzoylation of phenols/aromatic amines
6. Side chain oxidation of aromatic compounds
7. Diazo coupling reactions of aromatic amines
8. Bromination of anilides using green approach (Bromate-Bromide method)
9. Redox reaction including solid-phase method
10. Green 'multi-component-coupling' reaction
11. Selective reduction of *m*-dinitrobenzene to *m*-nitroaniline

**Students must also calculate percentage yield, based upon isolated yield (crude) and theoretical yield.**

B. Purification of the crude product is to be made by crystallisation from water/alcohol, crystallization after charcoal treatment, or sublimation, whichever is applicable.

C. Melting point of the purified product is to be noted.

#### **Reference Books**

1. Vogel, A. I. *Elementary Practical Organic Chemistry*, Part 1: *Small scale Preparations*, CBS Publishers and Distributors.
2. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009).
3. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. *Practical Organic Chemistry*, 5th Ed. Pearson (2012).
4. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
5. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015.

## SEMESTER-III

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### **CHEMISTRY -C V: PHYSICAL CHEMISTRY-II**

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

#### **Chemical Thermodynamics II**

(20 Lectures)

Second Law: Need for a Second law; statement of the second law of thermodynamics; Concept of heat reservoirs and heat engines; Carnot cycle; Physical concept of Entropy; Carnot engine and refrigerator; Kelvin – Planck and Clausius statements and equivalence of the two statements with entropic formulation; Carnot's theorem; Values of  $\int dQ/T$  and Clausius inequality; Entropy change of systems and surroundings for various processes and transformations; Entropy and unavailable work; Auxiliary state functions (G and A) and their variation with T, P and V. Criteria for spontaneity and equilibrium.

Thermodynamic relations: Maxwell's relations; Gibbs- Helmholtz equation, Joule-Thomson experiment and its consequences; inversion temperature; Joule-Thomson coefficient for a van der Waals gas; General heat capacity relations

#### **Applications of Thermodynamics – I**

(20 Lectures)

Partial properties and Chemical potential: Chemical potential and activity, partial molar quantities, relation between Chemical potential and Gibb's free energy and other thermodynamic state functions; variation of Chemical potential ( $\mu$ ) with temperature and pressure; Gibbs-Duhem equation; fugacity and fugacity coefficient; Variation of thermodynamic functions for systems with variable composition; Equations of states for these systems, Change in G, S H and V during mixing for binary solutions

Chemical Equilibrium: Thermodynamic conditions for equilibrium, degree of advancement; van't Hoff's reaction isotherm (deduction from chemical potential); Variation of free energy with degree of advancement; Equilibrium constant and standard Gibbs free energy change; Definitions of  $K_p$ ,  $K_C$  and  $K_X$ ; van't Hoff's reaction isobar and isochore from different standard states; Le Chatelier's principle and its derivation, variation of equilibrium constant under different conditions.

Nernst's distribution law; Application- (finding out  $K_{eq}$  using Nernst dist law for  $KI+I_2 = KI_3$  and dimerization of benzene. Solvent Extraction.

Chemical potential and other properties of ideal substances- pure and mixtures: a) Pure ideal gas-its Chemical potential and other thermodynamic functions and their changes during a change of; Thermodynamic parameters of mixing; Chemical potential of an ideal gas in an ideal gas mixture; Concept of standard states and choice of standard states of ideal gases

b) Condensed Phase – Chemical potential of pure solid and pure liquids, Ideal solution – Definition, Raoult's law; Mixing properties of ideal solutions, chemical potential of a component in an ideal solution; Choice of standard states of solids and liquids

### c) Foundation of Quantum Mechanics

(20 Lectures)

Beginning of Quantum Mechanics: Black body radiation, Wave-particle duality, light as particles: photoelectric and Compton effects; electrons as waves and the de Broglie hypothesis; Uncertainty relations (without proof)

Concept of Operators: Elementary concepts of operators, eigenfunctions and eigenvalues; Linear operators; Commutation of operators, commutator and uncertainty relation; Expectation value; Properties of Hermitian operator;

Wave function: Postulates of Quantum Mechanics, Schrodinger time-independent equation; nature of the equation, acceptability conditions for the wave functions and probability interpretations of wave function.

Particle in a box: Setting up of Schrodinger equation for one-dimensional box and its solution; Comparison with free particle eigenfunctions and eigenvalues. Properties of PB wave functions (normalisation, orthogonality, probability distribution); Expectation values of  $x$ ,  $x^2$ ,  $p_x$  and  $p_x^2$  and their significance in relation to the uncertainty principle; Extension of the problem to two and three dimensions and the concept of degenerate energy levels.

Simple Harmonic Oscillator: Setting up of One dimensional Schrödinger equation and discussion of solution and wave functions. Classical turning points, Expectation values of  $x$ ,  $x^2$ ,  $p_x$  and  $p_x^2$ .

#### Reference Books

1. Atkins, P. W. & Paula, J. de *Atkins', Physical Chemistry*, Oxford University Press
2. Castellan, G. W. *Physical Chemistry*, Narosa
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill
5. Rakshit, P.C., *Physical Chemistry*, Sarat Book House
6. Moore, W. J. *Physical Chemistry*, Orient Longman
7. Mortimer, R. G. *Physical Chemistry*, Elsevier
8. Denbigh, K. *The Principles of Chemical Equilibrium* Cambridge University Press
9. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
10. Levine, I. N. *Quantum Chemistry*, PHI
11. Atkins, P. W. *Molecular Quantum Mechanics*, Oxford
12. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill
13. Kapoor K.L, A Text Book Of Physical Chemistry ,McGrawHill, Volume II,IV
14. Sannigrahi A.B, Quantum Chemistry,2nd Edition,Books and Allied Pvt Ltd.
15. Klotz, I.M., Rosenberg, R. M. *Chemical Thermodynamics:Basic Concepts and Methods* Wiley
16. Glasstone, S. *An Introduction to Electrochemistry*, East-West Press

## **CHEMISTRY LAB-C V LAB**

**(60 Lectures)**

Experiment 1: Determination of heat of solution of oxalic acid from solubility measurement

Experiment 2: Determination of partition coefficient for the distribution of I<sub>2</sub> between water and CCl<sub>4</sub>

Experiment 3: Effect of ionic strength on the rate of Persulphate – Iodide reaction

Experiment 4: pH-metric titration of acid (mono- and di-basic) against strong base

Experiment 5: pH-metric titration of a tribasic acid against strong base.

Experiment 6: Kinetic study of inversion of cane sugar using a Polarimeter ( Preferably Digital)

### **Reference Books**

1. Viswanathan, B., Raghavan, P.S. *Practical Physical Chemistry* Viva Books (2009)
2. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson
3. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007)
4. Palit, S.R., De, S. K. *Practical Physical Chemistry* Science Book Agency
5. Levitt, B. P. edited *Findlay's Practical Physical Chemistry* Longman Group Ltd.
6. Gurtu, J. N., Kapoor, R., *Advanced Experimental Chemistry* S. Chand & Co. Ltd.
7. *Practical Workbook Chemistry (Honours), UGBS, Chemistry*, University of Calcutta, 2015

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## **CHEMISTRY -C VI: INORGANIC CHEMISTRY-II**

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

**Theory: 60 Lectures**

**Chemical Bonding-I**

**(20 Lectures)**

(i) *Ionic bond*: General characteristics, types of ions, size effects, radius ratio rule and its application and 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. Defects in solids (elementary idea). Solubility energetics of dissolution process

(ii) *Covalent bond*: Polarizing power and polarizability, ionic potential, Fajan's rules. Lewis structures, formal charge. Valence Bond Theory. The hydrogen molecule (Heitler-London approach), directional character of covalent bonds, hybridizations, equivalent and non-equivalent hybrid orbitals, Bent's rule, Dipole moments, VSEPR theory, shapes of molecules and ions containing lone pairs and bond pairs (examples from main groups chemistry) and multiple bonding ( $\sigma$  and  $\pi$  bond approach).

## Chemical Bonding-II

(20 Lectures)

(i) Molecular orbital concept of bonding (The approximations of the theory, Linear combination of atomic orbitals (LCAO)) (elementary pictorial approach): sigma and pi-bonds and delta interaction, multiple bonding. Orbital designations: *gerade*, *ungerade*, HOMO, LUMO. Orbital mixing,. MO diagrams of H<sub>2</sub>, Li<sub>2</sub>, Be<sub>2</sub>, B<sub>2</sub>, C<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, F<sub>2</sub>, and their ions wherever possible; Heteronuclear molecular orbitals: CO, NO, NO<sup>+</sup>, CN<sup>-</sup>, HF, BeH<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O. Bond properties: bond orders, bond lengths.

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

(iii) *Weak Chemical Forces*: Hydrogen bonding (theories of hydrogen bonding, valence bond treatment), receptor-guest interactions, Halogen bonds. Effects of chemical force, melting and boiling points.

## Chemistry of *s* and *p* Block Elements

(20 Lectures)

Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. 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. Beryllium hydrides and halides. Boric acid and borates, boron nitrides, borohydrides (diborane) and graphitic compounds, silanes, Oxides and oxoacids of nitrogen, phosphorus, sulphur and chlorine. Peroxo acids of sulphur, sulphur-nitrogen compounds, interhalogen compounds, polyhalide ions, pseudohalogens, fluorocarbons and basic properties of halogens.

### Reference Books

1. Lee, J. D. *Concise Inorganic Chemistry*, 5<sup>th</sup> Ed., Wiley India Pvt. Ltd., 2008.
2. 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.
3. Douglas, B.E. and McDaniel, D.H. *Concepts & Models of Inorganic Chemistry* Oxford, 1970.
4. Porterfield, H. W., *Inorganic Chemistry*, Second Edition, Academic Press, 2005.
5. Purecell, K.F. and Kotz, J.C., *An Introduction to Inorganic Chemistry*, Saunders: Philadelphia, 1980.
6. Cotton, F.A., Wilkinson, G., & Gaus, P.L. *Basic Inorganic Chemistry* 3<sup>rd</sup> Ed.; Wiley India.
7. Gillespie, R. J. and Hargittai, I., *The VSEPR Model of Molecular Geometry*, Prentice Hall (1992).
8. Albright, T., *Orbital interactions in chemistry*, John Wiley and Sons (2005).
9. Mingos, D.M.P., *Essential trends in inorganic chemistry*. Oxford University Press (1998).
10. Miessler, G. L., Fischer, P. J., Tarr, D. A., *Inorganic Chemistry*, Pearson, 5<sup>th</sup> Edition.
11. Kaplan, I., *Nuclear Physics*, Addison-Wesley Publishing Company Inc. London, 1964.
12. Friedlander, G., Kennedy, J. W., Macias, E. S. And Miller, J. M., *Nuclear and Radiochemistry*, Wiley, 1981.

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## **Core Course – VI (LAB)**

**(60 Lectures)**

### **Iodo-/ Iodimetric Titrations**

1. Estimation of Vitamin C
2. Estimation of (i) arsenite and (ii) antimony iodimetrically
3. Estimation of available chlorine in bleaching powder.

### **Estimation of metal content in some selective samples**

1. Estimation of Cu in brass.
2. Estimation of Cr and Mn in Steel.
3. Estimation of Fe in cement.

### **Reference Books**

1. Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis* 6th Ed., Pearson, 2009.
  2. *Practical Workbook Chemistry (Honours), UGBS, Chemistry, University of Calcutta*, 2015
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## **CHEMISTRY -C VII: ORGANIC CHEMISTRY-III**

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

**Theory: 60 Lectures**

### **Aromatic Substitution**

**(10 Lectures)**

*Electrophilic aromatic substitution:* mechanisms and evidences in favour of it; orientation and reactivity; reactions: nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reaction; one-carbon electrophiles (reactions: chloromethylation, Gatterman-Koch, Gatterman, Houben-Hoesch, Vilsmeier-Haack, Reimer-Tiemann, Kolbe-Schmidt); *Ips*o substitution.

*Nucleophilic aromatic substitution:* addition-elimination mechanism and evidences in favour of it; S<sub>N</sub>1 mechanism; cine substitution (benzyne mechanism), structure of benzyne.

### **Carbonyl and Related Compounds**

**(25 Lectures)**

*Addition to C=O:* structure, reactivity and preparation of carbonyl compounds; mechanism (with evidence), reactivity, equilibrium and kinetic control; Burgi-Dunitz



trajectory in nucleophilic additions; formation of hydrates, cyano hydrins and bisulphite adduct; nucleophilic addition-elimination reactions with alcohols, thiols and nitrogen-based nucleophiles; reactions: benzoin condensation, Cannizzaro and Tischenko reactions, reactions with ylides: Wittig and Corey-Chaykovsky reaction; Rupe rearrangement, oxidations and reductions: Clemmensen, Wolff-Kishner,  $\text{LiAlH}_4$ ,  $\text{NaBH}_4$ , MPV, Oppenauer, Bouveault-Blanc, acyloin condensation; oxidation of alcohols with PDC and PCC; periodic acid and lead tetraacetate oxidation of 1,2-diols.

*Exploitation of acidity of  $\alpha$ -H of  $\text{C}=\text{O}$ :* formation of enols and enolates; kinetic and thermodynamic enolates; reactions (mechanism with evidence): halogenation of carbonyl compounds under acidic and basic conditions, Hell-Volhard-Zelinsky (H. V. Z.) reaction, nitrosation,  $\text{SeO}_2$  (Riley) oxidation; condensations (mechanism with evidence): Aldol, Tollens', Knoevenagel, Claisen-Schmidt, Claisen ester including Dieckmann, Stobbe; Mannich reaction, Perkin reaction, Favorskii rearrangement; alkylation of active methylene compounds; preparation and synthetic applications of diethyl malonate and ethyl acetoacetate; specific enol equivalents (lithium enolates, enamines, aza-enolates and silyl enol ethers) in connection with alkylation, acylation and aldol type reaction.

*Elementary ideas of Green Chemistry:* Twelve (12) principles of green chemistry; planning of green synthesis; common organic reactions and their counterparts: reactions: Aldol, Friedel-Crafts, Michael, Knoevenagel, Cannizzaro, benzoin condensation and Dieckmann condensation.

*Nucleophilic addition to  $\alpha,\beta$ -unsaturated carbonyl system:* general principle and mechanism (with evidence); direct and conjugate addition, addition of enolates (Michael reaction), Stetter reaction, Robinson annulation.

*Substitution at  $sp^2$  carbon ( $\text{C}=\text{O}$  system):* mechanism (with evidence):  $B_{AC2}$ ,  $A_{AC2}$ ,  $A_{AC1}$ ,  $A_{AL1}$  (in connection to acid and ester); acid derivatives: amides, anhydrides & acyl halides (formation and hydrolysis including comparison).

## **Organometallics**

**(5 Lectures)**

*Grignard reagent; Organolithiums; Gilman cuprates:* preparation and reactions (mechanism with evidence); addition of Grignard and organolithium to carbonyl compounds; substitution on  $-\text{COX}$ ; directed ortho metalation of arenes using organolithiums, conjugate addition by Gilman cuprates; Corey-House synthesis; abnormal behavior of Grignard reagents; comparison of reactivity among Grignard, organolithiums and organocopper reagents; Reformatsky reaction; Blaise reaction; concept of *umpolung* and base-nucleophile dichotomy in case of organometallic reagents.

## **Nitrogen compounds**

**(10 Lectures)**

*Amines: Aliphatic & Aromatic:* preparation, separation (Hinsberg's method) and identification of primary, secondary and tertiary amines; reaction (with mechanism):

Eschweiler–Clarke methylation, diazo coupling reaction, Mannich reaction; formation and reactions of phenylenediamines, diazomethane and diazoacetic ester.

*Nitro compounds (aliphatic and aromatic):* preparation and reaction (with mechanism): reduction under different conditions; Nef carbonyl synthesis, Henry reaction and conjugate addition of nitroalkane anion.

*Alkyl nitrile and isonitrile:* preparation and reaction (with mechanism): Thorpe nitrile condensation, von Richter reaction.

*Diazonium salts and their related compounds:* reactions (with mechanism) involving replacement of diazo group; reactions: Gomberg, Meerwein, Japp-Klingermann.

## **Rearrangements**

**(10 Lectures)**

*Mechanism with evidence and stereochemical features for the following*

*Rearrangement to electron-deficient carbon:* Wagner-Meerwein rearrangement, pinacol rearrangement, dienone-phenol; Wolff rearrangement in Arndt-Eistert synthesis, benzil-benzilic acid rearrangement, Demjanov rearrangement, Tiffeneau–Demjanov rearrangement.

*Rearrangement to electron-deficient nitrogen:* rearrangements: Hofmann, Curtius, Lossen, Schmidt and Beckmann.

*Rearrangement to electron-deficient oxygen:* Baeyer-Villiger oxidation, cumene hydroperoxide-phenol rearrangement and Dakin reaction.

*Aromatic rearrangements: Migration from oxygen to ring carbon:* Fries rearrangement and Claisen rearrangement.

*Migration from nitrogen to ring carbon:* Hofmann-Martius rearrangement, Sommelet Houser rearrangement, Fischer-Hepp rearrangement, *N*-azo to *C*-azo rearrangement, Bamberger rearrangement, Orton rearrangement and benzidine rearrangement.

*Rearrangement reactions by green approach:* Fries rearrangement, Claisen rearrangement, Beckmann rearrangement, Baeyer-Villiger oxidation.

### **Reference Books**

1. Clayden, J., Greeves, N., Warren, S. *Organic Chemistry*, Second edition, Oxford University Press 2012.
2. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
3. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
4. Carey, F. A., Giuliano, R. M. *Organic Chemistry*, Eighth edition, McGraw Hill Education, 2012.
5. Loudon, G. M. *Organic Chemistry*, Fourth edition, Oxford University Press, 2008.
6. Norman, R.O. C., Coxon, J. M. *Principles of Organic Synthesis*, Third Edition, Nelson Thornes, 2003.

- Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
  - Finar, I. L. *Organic Chemistry (Volume 1)*, Pearson Education.
  - Graham Solomons, T.W., Fryhle, C. B. *Organic Chemistry*, John Wiley & Sons, Inc.
  - March, J. *Advanced Organic Chemistry*, Fourth edition, Wiley.
  - Jenkins, P. R., *Organometallic Reagents in Synthesis*, Oxford Chemistry Primer, Oxford University Press.
  - Ward, R. S., *Bifunctional Compounds*, Oxford Chemistry Primer, Oxford University Press.
  - Ahluwalia, V. K. *Strategies for Green Organic Synthesis*, ANE Books Pvt. Ltd.
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## **Core Course-VII (LAB)**

**(60 Lecturers)**

### **Experiment: Qualitative Analysis of Single Solid Organic Compounds**

- Detection of special elements (N, S, Cl, Br) by Lassaigne's test
- Solubility and classification (solvents: H<sub>2</sub>O, 5% HCl, 5% NaOH and 5% NaHCO<sub>3</sub>)
- Detection of the following functional groups by systematic chemical tests: aromatic amino (-NH<sub>2</sub>), aromatic nitro (-NO<sub>2</sub>), amido (-CONH<sub>2</sub>, including imide), phenolic -OH, carboxylic acid (-COOH), carbonyl (-CHO and >C=O); only one test for each functional group is to be reported.
- Melting point of the given compound
- Preparation, purification and melting point determination of a crystalline derivative of the given compound.
- Identification of the compound through literature survey.

Each student, during laboratory session, is required to carry out qualitative chemical tests for all the special elements and the functional groups with relevant derivatisation in known and unknown (**at least six**) organic compounds.

### **Reference Books**

- Vogel, A. I. *Elementary Practical Organic Chemistry*, Part 2: *Qualitative Organic Analysis*, CBS Publishers and Distributors..
  - Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009).
  - Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. *Practical Organic Chemistry*, 5th Ed., Pearson (2012).
  - Clarke, H. T., *A Handbook of Organic Analysis (Qualitative and Quantitative)*, Fourth Edition, CBS Publishers and Distributors (2007).
  - Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015.
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## SEMESTER-IV

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### **CHEMISTRY -C VIII: PHYSICAL CHEMISTRY-III**

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

**Theory: 60 Lectures**

**Application of Thermodynamics – II**

**(20 lectures)**

**Colligative properties:** Vapour pressure of solution; Ideal solutions, ideally diluted solutions and colligative properties; Raoult's law; Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) Osmotic pressure] and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution; Abnormal colligative properties.

**Phase Equilibrium:** Definitions of phase, component and degrees of freedom; Phase rule and its derivations; Definition of phase diagram; Phase diagram for water, CO<sub>2</sub>, Sulphur.

First order phase transition and Clapeyron equation; Clausius-Clapeyron equation - derivation and use; Ehrenfest Classification of phase transition.

**Binary solutions:** Liquid vapour equilibrium for two component systems Ideal solution at fixed temperature and pressure; Principle of fractional distillation; Duhem-Margules equation; Henry's law; Konowaloff's rule; Positive and negative deviations from ideal behaviour; Azeotropic solution; Liquid-liquid phase diagram using phenol- water system; Solid-liquid phase diagram; Eutectic mixture

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

**ELECTROCHEMISTRY:**

**(15 Lectures)**

**(i) Conductance and transport number**

Ion conductance; Conductance and measurement of conductance, cell constant, specific conductance and molar conductance; Variation of specific and equivalent conductance with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions; Equivalent and molar conductance at infinite dilution and their determination for strong and weak electrolytes; Debye -Huckel theory of Ion atmosphere (qualitative)-asymmetric effect, relaxation effect and electrophoretic effect; Debye-Huckel limiting law-brief qualitative description. Estimation of activity coefficient for electrolytes using Debye-Huckel limiting law. Primary Kinetic Salt Effect. Ostwald's dilution law; Ionic mobility; Application of conductance measurement (determination of solubility product and ionic product of water); Conductometric titrations Transport number, Principles of Hittorf's and Moving-boundary method; Wien effect, Debye-Falkenhagen effect, Walden's rule

**(ii) Electromotive Force:** Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials; Chemical cells, reversible and irreversible cells with examples; Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and  $\text{SbO/Sb}_2\text{O}_3$  electrodes  
Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers; Potentiometric titrations (acid-base, redox, precipitation)

### **Crystal Structure**

**(20 Lectures)**

Bravais Lattice and Laws of Crystallography: Types of solid, Bragg's law of diffraction; Laws of crystallography (Haüy's law and Steno's law); Permissible symmetry axes in crystals; Lattice, space lattice, unit cell, crystal planes, Bravais lattice. Packing of uniform hard sphere, close packed arrangements (fcc and hcp); Tetrahedral and octahedral voids. Void space in p-type, F-type and I-type cubic systems

Crystal planes: Distance between consecutive planes [cubic, tetragonal and orthorhombic lattices]; Indexing of planes, Miller indices; calculation of  $d_{hkl}$ ; Relation between molar mass and unit cell dimension for cubic system; Bragg's law (derivation). Determination of crystal structure: Powder method; Structure of NaCl and KCl crystals.

Specific heat of solid: Coefficient of thermal expansion, thermal compressibility of solids; Dulong –Petit's law; Perfect Crystal model, Einstein's theory – derivation from partition function, limitations; Debye's  $T^3$  law – analysis at the two extremes

**(05 Lectures)**

Dipole moment and polarizability: Polarizability of atoms and molecules, dielectric constant and polarisation, molar polarisation for polar and non-polar molecules; Clausius-Mosotti equation and Debye equation (both without derivation) and their application; Determination of dipole moments

### **Reference Books**

1. Castellan, G. W. *Physical Chemistry*, Narosa
2. Atkins, P. W. & Paula, J. de *Atkins', Physical Chemistry*, Oxford University Press
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill
5. Moore, W. J. *Physical Chemistry*, Orient Longman
6. Mortimer, R. G. *Physical Chemistry*, Elsevier
7. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
8. Levine, I. N. *Quantum Chemistry*, 7th Edition, Pearson India
9. Atkins, P. W. *Molecular Quantum Mechanics*, Oxford

10. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
11. Maron, S.H., Prutton, C. F., *Principles of Physical Chemistry*, McMillan
12. Klotz, I.M., Rosenberg, R. M. *Chemical Thermodynamics: Basic Concepts and Methods* Wiley
13. Glasstone, S. An Introduction to Electrochemistry, East-West Press
14. Kapoor K.L, A Text Book Of Physical Chemistry ,McGrawHill, Volume I,III
15. Sannigrahi A.B, Quantum Chemistry,2nd Edition,Books and Allied Pvt Ltd

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### **Core Course – X (LAB)**

**(60 Lectures)**

**Experiment 1:** Potentiometric titration of Mohr's salt solution against standard  $K_2Cr_2O_7$  solution

**Experiment 2:** Conductometric titration of an acid (strong, weak/ monobasic, dibasic, and acid mixture ) against strong base.

**Experiment 3:** Study of saponification reaction conductometrically

**Experiment 4:** Verification of Ostwald's dilution law and determination of  $K_a$  of weak acid

**Experiment 5:** Determination of  $K_{sp}$  for AgCl by potentiometric titration of  $AgNO_3$  solution against standard KCl solution

**Experiment 6:** Study of phenol-water phase diagram

### **Reference Books**

1. Viswanathan, B., Raghavan, P.S. *Practical Physical Chemistry* Viva Books (2009)
2. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson
3. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007)
4. Palit, S.R., De, S. K. *Practical Physical Chemistry* Science Book Agency
5. Levitt, B. P. edited *Findlay's Practical Physical Chemistry* Longman Group Ltd.
6. Gurtu, J. N., Kapoor, R., *Advanced Experimental Chemistry* S. Chand & Co. Ltd.
7. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015

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### **CHEMISTRY -C IX: INORGANIC CHEMISTRY-III**

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

**Theory: 60 Lectures**

**Noble Gases:**

**(10 Lectures)**

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> and XeF<sub>4</sub>). Xenon-oxygen compounds. Molecular shapes of noble gas compounds (VSEPR theory).

**Inorganic Polymers: (08 Lectures)**

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

**Coordination Chemistry-I (15 Lectures)**

Coordinate bonding: double and complex salts. Werner's theory of coordination complexes, Classification of ligands, Ambidentate ligands, chelates, Coordination numbers, IUPAC nomenclature of coordination complexes (up to two metal centers), Isomerism in coordination compounds, constitutional and stereo isomerism, Geometrical and optical isomerism in square planar and octahedral complexes.

**Coordination Chemistry-II (27 Lectures)**

VB description and its limitations. Elementary Crystal Field Theory: splitting of d<sup>n</sup> configurations in octahedral, square planar and tetrahedral fields, crystal field stabilization energy (CFSE) in weak and strong fields; pairing energy. Spectrochemical series. Jahn-Teller distortion. Octahedral site stabilization energy (OSSE). Metal-ligand bonding (MO concept, elementary idea), sigma- and pi-bonding in octahedral complexes (qualitative pictorial approach) and their effects on the oxidation states of transitional metals (examples). Magnetism and Colour: Orbital and spin magnetic moments, spin only moments of d<sup>n</sup> ions and their correlation with effective magnetic moments, including orbital contribution; quenching of magnetic moment: super exchange and antiferromagnetic interactions (elementary idea with examples only); d-d transitions; L-S coupling; qualitative Orgel diagrams for 3d<sup>1</sup> to 3d<sup>9</sup> ions. Racah parameter. Selection rules for electronic spectral transitions; spectrochemical series of ligands; charge transfer spectra (elementary idea).

**Reference Books**

1. 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.
2. Greenwood, N.N. & Earnshaw A. *Chemistry of the Elements*, Butterworth-Heinemann, 1997.
3. Cotton, F.A., Wilkinson, G., Murrillo, C. A., Bochmann, M., *Advanced Inorganic Chemistry 6<sup>th</sup> Ed.* 1999., Wiley.
4. Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry 4<sup>th</sup> Ed.*, Pearson, 2010.
5. Purecell, K.F. and Kotz, J.C., *An Introduction to Inorganic Chemistry*, Saunders: Philadelphia, 1980.
6. Mingos, D.M.P., *Essential trends in inorganic chemistry*. Oxford University Press (1998).

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## **Core Course – VIII (LAB)**

**(60 Lectures)**

### **Complexometric titration**

1. Zn(II)
2. Zn(II) in a Zn(II) and Cu(II) mixture.
3. Ca(II) and Mg(II) in a mixture.
4. Hardness of water.

### **Inorganic preparations**

1.  $[\text{Cu}(\text{CH}_3\text{CN})_4]\text{PF}_6/\text{ClO}_4$
2. *Cis* and *trans*  $\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$
3. Potassium diaquadioxalatochromate(III)
4. Tetraamminecarbonatocobalt (III) ion
5. Potassium tris(oxalato)ferrate(III)
6. Tris-(ethylenediamine) nickel(II) chloride.
7.  $[\text{Mn}(\text{acac})_3]$  and  $[\text{Fe}(\text{acac})_3]$  (acac= acetylacetonate)

### **Reference Books**

1. Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis* 6th Ed., Pearson, 2009.
  2. *Inorganic Synthesis*, Vol. 1-10.
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## **CHEMISTRY -C X: ORGANIC CHEMISTRY-IV**

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

**Theory: 60 Lectures**

### **The Logic of Organic Synthesis**

**(14 Lectures)**

*Retrosynthetic analysis:* disconnections; synthons, donor and acceptor synthons; natural reactivity and *umpolung*; latent polarity in bifunctional compounds: consonant and dissonant polarity; illogical electrophiles and nucleophiles; synthetic equivalents; functional group interconversion and addition (FGI and FGA); C-C disconnections and synthesis: one-group and two-group (1,2- to 1,5-dioxygenated compounds), reconnection (1,6-dicarbonyl); protection-deprotection strategy (alcohol, amine, carbonyl, acid).

*Strategy of ring synthesis:* thermodynamic and kinetic factors; synthesis of large rings, application of high dilution technique.



*Asymmetric synthesis*: stereoselective and stereospecific reactions; diastereoselectivity and enantioselectivity (only definition); enantioselectivity: kinetically controlled MPV reduction; diastereoselectivity: addition of nucleophiles to C=O adjacent to a stereogenic centre: Felkin-Anh and Zimmermann-Traxler models.

**(12 Lectures)**

***Polynuclear hydrocarbons and their derivatives***: synthetic methods include Haworth, Bardhan-Sengupta, Bogert-Cook and other useful syntheses (with mechanistic details); fixation of double bonds and Fries rule; reactions (with mechanism) of naphthalene, anthracene, phenanthrene and their derivatives.

***Heterocyclic compounds***: 5- and 6-membered rings with one heteroatom; reactivity, orientation and important reactions (with mechanism) of furan, pyrrole, thiophene and pyridine; synthesis (including retrosynthetic approach and mechanistic details): pyrrole: Knorr synthesis, Paal-Knorr synthesis, Hantzsch; furan: Paal-Knorr synthesis, Feist-Benary synthesis and its variation; thiophenes: Paal-Knorr synthesis, Hinsberg synthesis; pyridine: Hantzsch synthesis; benzo-fused 5- and 6-membered rings with one heteroatom: reactivity, orientation and important reactions (with mechanistic details) of indole, quinoline and isoquinoline; synthesis (including retrosynthetic approach and mechanistic details): indole: Fischer, Madelung and Reissert; quinoline: Skraup, Doebner- Miller, Friedlander; isoquinoline: Bischler-Napieralski synthesis.

### **Alkaloids**

**(8 Lectures)**

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

### **Terpenes**

**(6 Lectures)**

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

### **Organic Spectroscopy**

**(20 Lectures)**

*UV Spectroscopy*: introduction; types of electronic transitions, end absorption; transition dipole moment and allowed/forbidden transitions; chromophores and auxochromes; Bathochromic and Hypsochromic shifts; intensity of absorptions (Hyper-/Hypochromic effects); application of Woodward's Rules for calculation of  $\lambda_{\max}$  for the following systems: conjugated diene,  $\alpha,\beta$ -unsaturated aldehydes and ketones (alicyclic, homoannular and heteroannular); extended conjugated systems (dienes, aldehydes and ketones); relative positions of  $\lambda_{\max}$  considering conjugative effect, steric effect, solvent effect, effect of pH; effective chromophore concentration: keto-enol systems; benzenoid transitions.

*IR Spectroscopy*: introduction; modes of molecular vibrations (fundamental and non-fundamental); IR active molecules; application of Hooke's law, force constant;

*fingerprint region* and its significance; effect of deuteration; overtone bands; vibrational coupling in IR; characteristic and diagnostic stretching frequencies of C-H, N-H, O-H, C-O, C-N, C-X, C=C (including skeletal vibrations of aromatic compounds), C=O, C=N, N=O, C≡C, C≡N; characteristic/diagnostic bending vibrations are included; factors affecting stretching frequencies: effect of conjugation, electronic effects, mass effect, bond multiplicity, ring-size, solvent effect, H-bonding on IR absorptions; application in functional group analysis.

*NMR Spectroscopy*: introduction; nuclear spin; NMR active molecules; basic principles of Proton Magnetic Resonance; equivalent and non-equivalent protons; chemical shift and factors influencing it; ring current effect; significance of the terms: up-/downfield, shielded and deshielded protons; spin coupling and coupling constant (1st order spectra); relative intensities of *first-order* multiplets: Pascal's triangle; chemical and magnetic equivalence in NMR ; elementary idea about *non-first-order* splitting; anisotropic effects in alkene, alkyne, aldehydes and aromatics; NMR peak area, integration; relative peak positions with coupling patterns of common organic compounds (both aliphatic and benzenoid-aromatic); rapid proton exchange; interpretation of NMR spectra of simple compounds.

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

#### **Reference Books**

1. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Norman, R.O. C., Coxon, J. M. *Principles of Organic Synthesis*, Third Edition, Nelson Thornes, 2003.
4. Clayden, J., Greeves, N., Warren, S., *Organic Chemistry*, Second edition, Oxford University Press 2012.
5. Silverstein, R. M., Bassler, G. C., Morrill, T. C. *Spectrometric Identification of Organic Compounds*, John Wiley and Sons, INC, Fifth edition.
6. Kemp, W. *Organic Spectroscopy*, Palgrave.
7. Pavia, D. L. *et al. Introduction to Spectroscopy*, 5th Ed. Cengage Learning India Ed. (2015).
8. Dyer, J. *Application of Absorption Spectroscopy of Organic Compounds*, PHI Private Limited
9. March, J. *Advanced Organic Chemistry*, Fourth edition, Wiley.
10. Harwood, L. M., *Polar Rearrangements*, Oxford Chemistry Primer, Oxford University Press.
11. Bailey, Morgan, *Organonitrogen Chemistry*, Oxford Chemistry Primer, Oxford University Press.
12. Ahluwalia, V. K. *Strategies for Green Organic Synthesis*, ANE Books Pvt. Ltd.
13. Warren, S. *Organic Synthesis the Disconnection Approach*, John Wiley and Sons.
14. Warren, S., *Designing Organic Synthesis*, Wiley India, 2009.

15. Carruthers, W. *Modern methods of Organic Synthesis*, Cambridge University Press.
  16. Willis, C. A., Wills, M., *Organic Synthesis*, Oxford Chemistry Primer, Oxford University Press.
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### **Core Course-IX (LAB)**

**(60 Lectures)**

**Quantitative Estimations:** Each student is required to perform all the experiments [ ANY five will be set in the examination]

1. Estimation of glycine by Sørensen's formol method
2. Estimation of glucose by titration using Fehling's solution
3. Estimation of sucrose by titration using Fehling's solution
4. Estimation of aromatic amine (aniline) by bromination (Bromate-Bromide) method
5. Estimation of acetic acid in commercial vinegar
6. Estimation of urea (hypobromite method)
7. Estimation of saponification value of oil/fat/ester

#### **Reference Books**

1. Arthur, I. V. *Quantitative Organic Analysis*, Pearson
  2. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015
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# SEMESTER-V

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## **CHEMISTRY -C XI: PHYSICAL CHEMISTRY-IV**

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

**Theory: 60 Lectures**

### **Quantum Chemistry II**

**(30 Lectures)**

**Angular momentum**: Commutation rules, quantization of square of total angular momentum and z-component; Rigid rotator model of rotation of diatomic molecule; Schrödinger equation, transformation to spherical polar coordinates; Separation of variables. Spherical harmonics; Discussion of solution

**Hydrogen atom and hydrogen-like ions**: Setting up of Schrödinger equation in spherical polar coordinates, Separation of variables, Solution of angular Part ( $\phi$  part only ) radial part, quantization of energy (only final energy expression); Real wave functions. Average and most probable distances of electron from nucleus; Setting up of Schrödinger equation for many-electron atoms (He, Li) Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

**LCAO** : Born-Oppenheimer approximation. Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of  $H_2^+$ ; Bonding and antibonding orbitals; Qualitative extension to  $H_2$ ; Comparison of LCAO-MO and VB treatments of  $H_2$  and their limitations. (only wave functions, detailed solution not required) and their limitations.

### **Statistical Thermodynamics**

**(20 Lectures)**

**Configuration**: Macrostates, microstates and configuration; calculation with harmonic oscillator; variation of W with E; equilibrium configuration

**Boltzmann distribution**: Thermodynamic probability, entropy and probability, Boltzmann distribution formula (with derivation); Applications to barometric distribution; Partition function, concept of ensemble - canonical ensemble and grand canonical ensembles

**Partition function**: molecular partition function and thermodynamic properties, Maxwell's speed distribution; Gibbs' paradox

**3<sup>rd</sup> law**: Absolute entropy, Planck's law, Calculation of entropy, Nernst heat theorem

**Adiabatic demagnetization**: Approach to zero Kelvin, adiabatic cooling, demagnetization, adiabatic demagnetization – involved curves

### **Numerical Analysis**

**(10 Lectures)**

Roots of Equation: Numerical methods for finding the roots of equations: Quadratic Formula, Iterative Methods (e.g., Newton Raphson Method).

Least-Squares Fitting. Numerical Differentiation. Numerical Integration( Trapezoidal and Simpson's Rule)

### **Reference Books**

1. Castellan, G. W. *Physical Chemistry*, Narosa
2. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill
3. Moore, W. J. *Physical Chemistry*, Orient Longman
4. Atkins, P. W. & Paula, J. de *Atkins', Physical Chemistry*, Oxford University Press
5. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
6. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
7. Nash, L. K. *Elements of Statistical Thermodynamics*, Dover
8. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill
9. Billmeyer, F. W. *Textbook of Polymer Science*, John Wiley & Sons, Inc.
10. Seymour, R. B. & Carraher, C. E. *Polymer Chemistry: An Introduction*, Marcel Dekker, Inc.
11. Odian, G. *Principles of Polymerization*, Wiley
12. Billmeyer, F. W. *Textbook of Polymer Science*, Wiley Interscience, 1971.
13. V. Rajaraman, *Computer Oriented Numerical Methods*, PHI Learning, 2013
14. V. Rajaraman, *Computer Programming in FORTRAN 77*, Prentice Hall, 1997
15. Martin Cwiakala, *Schaum's Outline of Programming with FORTRAN 77*, 1995
16. Sannigrahi A.B, *Quantum Chemistry*, 2nd Edition, Books and Allied Pvt Ltd
  
17. Levine, I. N. *Quantum Chemistry*, 7th Edition, Pearson India

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### **Core Course-XI (LAB)** **(60 Lectures)**

Computer programs(Using FORTRAN or C) based on numerical methods for

Programming 1: Roots of equations: (e.g. volume of van der Waals gas and comparison with ideal gas, pH of a weak acid)

Programming 2: Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations)

Programming 3: Numerical integration (e.g. entropy/ enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values

### **Reference Books**

1. McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008)
2. Mortimer, R. *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier (2005)
3. Yates, P. *Chemical Calculations*. 2nd Ed. CRC Press (2007)
4. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5
5. Let us C, Yashvant Kanetkar, BPB Publication, 15th Edition, 2016

## **CHEMISTRY -C XII: ORGANIC CHEMISTRY-V**

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

**Theory: 60 Lectures**

### **Pericyclic reactions**

**(8 Lectures)**

*Mechanism, stereochemistry, regioselectivity in case of*

*Electrocyclic reactions:* FMO approach involving  $4\pi$ - and  $6\pi$ -electrons (thermal and photochemical) and corresponding cycloreversion reactions.

*Cycloaddition reactions:* FMO approach, Diels-Alder reaction, photochemical [2+2] cycloadditions.

*Sigmatropic reactions:* FMO approach, sigmatropic shifts and their order; [1,3]- and [1,5]-H shifts and [3,3]-shifts with reference to Claisen and Cope rearrangements.

### **Cyclic Stereochemistry**

**(8 Lectures)**

*Alicyclic compounds:* concept of I-strain; conformational analysis: cyclohexane, mono and disubstituted cyclohexane; symmetry properties and optical activity; topomerisation; ring-size and ease of cyclisation; conformation & reactivity in cyclohexane system: consideration of steric and stereoelectronic requirements; elimination (E2, E1), nucleophilic substitution ( $S_N1$ ,  $S_N2$ ,  $S_{Ni}$ , NGP), merged substitution-elimination; rearrangements; oxidation of cyclohexanol, esterification, saponification, lactonisation, epoxidation, pyrolytic *syn* elimination and fragmentation reactions.

### **Carbohydrates**

**(12 Lectures)**

*Monosaccharides:* Aldoses up to 6 carbons; structure of D-glucose & D-fructose (configuration & conformation); ring structure of monosaccharides (furanose and pyranose forms): Haworth representations and non-planar conformations; anomeric effect (including stereoelectronic explanation); mutarotation; epimerization; reactions (mechanisms in relevant cases): Fischer glycosidation, osazone formation, bromine-water oxidation,  $HNO_3$  oxidation, selective oxidation of terminal  $-CH_2OH$  of aldoses, reduction to alditols, Lobry de Bruyn-van Ekenstein rearrangement; stepping-up (Kiliani-Fischer method) and stepping-down (Ruff's & Wohl's methods) of aldoses; end-group-interchange of aldoses; acetonide (isopropylidene) and benzylidene protections; ring-size determination; Fischer's proof of configuration of (+)-glucose.

*Disaccharides:* Glycosidic linkages, concept of glycosidic bond formation by glycosyl donor-acceptor; structure of sucrose, inversion of cane sugar.

*Polysaccharides:* starch (structure and its use as an indicator in titrimetric analysis).

### **Biomolecules**

**(14 Lectures)**

*Amino acids:* synthesis with mechanistic details: Strecker, Gabriel, acetamido malonic ester, azlactone, Bücherer hydantoin synthesis, synthesis involving diketopiperazine; isoelectric point, zwitterions; electrophoresis, reaction (with mechanism): ninhydrin reaction, Dakin-West reaction; resolution of racemic amino acids.

*Peptides*: peptide linkage and its geometry; syntheses (with mechanistic details) of peptides using *N*-protection & *C*-protection, solid-phase (Merrifield) synthesis; peptide sequence: *C*-terminal and *N*-terminal unit determination (Edman, Sanger & 'dansyl' methods); partial hydrolysis; specific cleavage of peptides: use of CNBr.

*Nucleic acids*: pyrimidine and purine bases (only structure & nomenclature); nucleosides and nucleotides corresponding to DNA and RNA; mechanism for acid catalysed hydrolysis of nucleosides (both pyrimidine and purine types); comparison of alkaline hydrolysis of DNA and RNA; elementary idea of double helical structure of DNA (Watson-Crick model); complimentary base-pairing in DNA.

### **Concept of Energy in Biosystems**

**(12 Lectures)**

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<sup>+</sup>, FAD.

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

Overview of catabolic pathways of fat and protein.

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

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

### **Pharmaceutical Compounds: Structure and Importance**

**(6 Lectures)**

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).

### **Reference Books**

1. Clayden, J., Greeves, N., Warren, S. *Organic Chemistry*, Second edition, Oxford University Press 2012.
2. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London.
3. Nasipuri, D. *Stereochemistry of Organic Compounds*, Wiley Eastern Limited.
4. Fleming, I. *Molecular Orbitals and Organic Chemical reactions*, Reference/Student Edition, Wiley, 2009.
5. Fleming, I. *Pericyclic Reactions*, Oxford Chemistry Primer, Oxford University Press.
6. Gilchrist, T. L. & Storr, R. C. *Organic Reactions and Orbital symmetry*, Cambridge University Press.

7. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
8. Finar, I. L. *Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
9. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
10. Loudon, G. M. *Organic Chemistry*, Fourth edition, Oxford University Press.
11. James, J., Peach, J. M. *Stereochemistry at a Glance*, Blackwell Publishing, 2003.
12. Robinson, M. J. T., *Stereochemistry*, Oxford Chemistry Primer, Oxford University Press, 2005.
13. Davis, B. G., Fairbanks, A. J., *Carbohydrate Chemistry*, Oxford Chemistry Primer, Oxford University Press.
14. Joule, J. A. Mills, K. *Heterocyclic Chemistry*, Blackwell Science.
15. Acheson, R.M. *Introduction to the Chemistry of Heterocyclic compounds*, John Wiley & Sons (1976).
16. Gilchrist, T. L. *Heterocyclic Chemistry*, 3rd edition, Pearson.
17. Davies, D. T., *Heterocyclic Chemistry*, Oxford Chemistry Primer, Oxford University Press.

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## **Core Course-XII (LAB)**

**(60 Lectures)**

### **A. Chromatographic Separations**

1. TLC separation of a mixture containing 2/3 amino acids
2. TLC separation of a mixture of dyes (fluorescein and methylene blue)
3. Column chromatographic separation of leaf pigments from spinach leaves
4. Column chromatographic separation of mixture of dyes
5. Paper chromatographic separation of a mixture containing 2/3 amino acids
6. Paper chromatographic separation of a mixture containing 2/3 sugars

### **B. Spectroscopic Analysis of Organic Compounds**

1. Assignment of labelled peaks in the  $^1\text{H}$  NMR spectra of the known organic compounds explaining the relative  $\delta$ -values and splitting pattern.
2. Assignment of labelled peaks in the IR spectrum of the same compound explaining the relative frequencies of the absorptions (C-H, O-H, N-H, C-O, C-N, C-X, C=C, C=O, N=O, C $\equiv$ C, C $\equiv$ N stretching frequencies; **characteristic bending vibrations are included**).
3. The students must record full spectral analysis of **at least 15 (fifteen)** compounds from the following list:



(i) 4'-Bromoacetanilide (ii) 2-Bromo-4'-methylacetophenone (iii) Vanillin (iv) 2'-Methoxyacetophenone (v) 4-Aminobenzoic acid (vi) Salicylamide (vii) 2'-Hydroxyacetophenone (viii) 1,3-Dinitrobenzene (ix) *trans*-Cinnamic acid (x) Diethyl fumarate (xi) 4-Nitrobenzaldehyde (xii) 4'-Methylacetanilide (xiii) Mesityl oxide (xiv) 2-Hydroxybenzaldehyde (xv) 4-Nitroaniline (xvi) 2,3-Dimethylbenzotrile (xvii) Pent-1-yn-3-ol (xviii) 3-Nitrobenzaldehyde (xix) 3-Aminobenzoic acid (xx) Ethyl 3-aminobenzoate (xxi) Ethyl 4-aminobenzoate (xxii) 3-nitroanisole

### **Reference Books**

1. *Practical Workbook Chemistry (Honours), UGBS, Chemistry*, University of Calcutta, 2015
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012).
3. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education.

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## **SEMESTER-VI**

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### **CHEMISTRY -C XIII: INORGANIC CHEMISTRY-IV**

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

**Theory: 60 Lectures**

#### **Chemistry of d- and f- block elements (15 Lectures)**

##### **Transition Elements:**

General comparison of 3d, 4d and 5d elements in term of electronic configuration, oxidation states, redox properties, coordination chemistry.

##### **Lanthanoids and Actinoids:**

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

#### **Reaction Kinetics and Mechanism (15 Lectures)**

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans- effect and its application in complex synthesis, 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.

#### **General Principles of Metallurgy (10 Lectures)**

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

#### **Elemental analysis: (10 Lectures)**

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).

#### **Electroanalytical Methods: (05 Lectures)**

Potentiometry & Voltammetry

**X-ray analysis and electron spectroscopy (surface analysis): (05 Lectures)**  
**Elementary idea**

**Core Course-XIII(LAB)**  
**(60 Lectures)**

**Gravimetry**

1. Estimation of Ni(II) using Dimethylglyoxime (DMG).
2. Estimation of copper as CuSCN.
3. Estimation of Al(III) by precipitating with oxine and weighing as Al(oxine)<sub>3</sub> (aluminium oxinate).
4. Estimation of chloride.

**Instrumental Techniques**

1. Measurement of <sup>10</sup>Dq by spectrophotometric method.
2. Determination of  $\lambda_{\max}$  of [Mn(acac)<sub>3</sub>] and [Fe(acac)<sub>3</sub>] complexes.
3. Potentiometric Titration of a Chloride-Iodide Mixture
4. Cyclic Voltammetry of the Ferrocyanide/ Ferricyanide Couple

**Chromatography of metal ions**

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

1. Ni (II) and Co (II)
2. Fe (III) and Al (III)

**Reference Books**

1. Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis* 6th Ed., Pearson, 2009.
2. Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Ed.
3. Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. *Instrumental Methods of Analysis*, 7<sup>th</sup> Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988

## **CHEMISTRY -C XIV: PHYSICAL CHEMISTRY-V**

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

**Theory: 60 Lectures**

### **a) Molecular Spectroscopy (30 Lectures)**

Interaction of electromagnetic radiation with molecules and various types of spectra; **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; Diatomic vibrating rotator, P, Q, R branches

**Electronic Spectroscopy**: Potential energy curves (diatomic molecules), Frank-Condon principle and vibrational structure of electronic spectra; Bond dissociation and principle of determination of dissociation energy (ground state); Decay of excited states by radiative and non-radiative paths; Pre-dissociation; Fluorescence and phosphorescence, Jablonskii diagram;

**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

**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

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

### **b) Photochemistry (10 Lectures)**

**Lambert-Beer's law**: Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients; Laws of photochemistry, Stark-Einstein law of photochemical equivalence quantum yield, actinometry, examples of low and high quantum yields

**Rate of Photochemical processes**: Photochemical equilibrium and the differential rate of photochemical reactions, Photostationary state; HI decomposition, H<sub>2</sub>-Br<sub>2</sub> reaction, dimerisation of anthracene; photosensitised reactions, quenching; Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence

### **c) Surface phenomenon (20 Lectures)**

**Surface tension and energy**: Surface tension, surface energy, excess pressure, capillary rise and surface tension; Work of cohesion and adhesion, spreading of liquid over other surface; Vapour pressure over curved surface; Temperature dependence of surface tension

Adsorption: Physical and chemical adsorption; Freundlich and Langmuir adsorption isotherms; multilayer adsorption and BET isotherm (no derivation required); Gibbs adsorption isotherm and surface excess; Heterogenous catalysis (single reactant); Zero order and fractional order reactions;

Colloids: Lyophobic and lyophilic sols, Origin of charge and stability of lyophobic colloids, Coagulation and Schultz-Hardy rule, Zeta potential and Stern double layer (qualitative idea), Tyndall effect; Electrokinetic phenomena (qualitative idea only); Determination of Avogadro number by Perrin's method; Stability of colloids and zeta potential; Micelle formation

### Reference Books

1. Castellan, G. W. Physical Chemistry, Narosa
2. Levine, I. N. Physical Chemistry, Tata McGraw-Hill
3. Atkins, P. W. & Paula, J. de Atkin's, Physical Chemistry, Oxford University Press
4. McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press
5. Mortimer, R. G. Physical Chemistry, Elsevier
6. Laidler, K. J. Chemical Kinetics, Pearson
7. Banwell, C. N. Fundamentals of Molecular Spectroscopy, Tata-McGraw-Hill
8. Barrow, G. M. Molecular Spectroscopy, McGraw-Hill
9. Hollas, J.M. Modern Spectroscopy, Wiley India
10. McHale, J. L. Molecular Spectroscopy, Pearson Education
11. Wayne, C. E. & Wayne, R. P. Photochemistry, OUP
12. Brown, J. M. Molecular Spectroscopy, OUP
13. Levine, I. N. *Quantum Chemistry*, 7th Edition, Pearson India
  
14. Atkins, P. W. *Molecular Quantum Mechanics*, 5th Edition Oxford

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### Core Course – XIV (LAB)

(60 Lectures)

Experiment 1: Determination of surface tension of a liquid using Stalagmometer

Experiment 2: Determination of CMC from surface tension measurements

Experiment 3: Verification of Beer and Lambert's Law for  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  solution

Experiment 4: Study of kinetics of  $\text{K}_2\text{S}_2\text{O}_8 + \text{KI}$  reaction, spectrophotometrically

Experiment 5: Determination of pH of unknown buffer, spectrophotometrically

Experiment 6: Spectrophotometric determination of CMC

### Reference Books

1. Viswanathan, B., Raghavan, P.S. *Practical Physical Chemistry* Viva Books (2009)
  2. Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis* 6th Ed., Pearson
  3. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007)
  4. Palit, S.R., De, S. K. *Practical Physical Chemistry* Science Book Agency
  5. Levitt, B. P. edited *Findlay's Practical Physical Chemistry* Longman Group Ltd.
  6. Gurtu, J. N., Kapoor, R., *Advanced Experimental Chemistry* S. Chand & Co. Ltd.
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## **DSE-1: ADVANCED INORGANIC CHEMISTRY**

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

### **Theoretical Principles in Qualitative Analysis**

(10 Lectures)

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.

### **Bioinorganic Chemistry**

(25 Lectures)

Elements of life: essential and beneficial elements, major, trace and ultratrace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Fe}^{3+/2+}$ ,  $\text{Cu}^{2+/+}$ , and  $\text{Zn}^{2+}$ ). Metal ion transport across biological membrane  $\text{Na}^+/\text{K}^+$ -ion pump. Dioxygen molecule in life. Dioxygen management proteins: Haemoglobin, Myoglobin, Hemocyanine and Hemerythrin. Electron transfer proteins: Cytochromes and Ferredoxins. Hydrolytic enzymes: carbonate bicarbonate buffering system and carbonic anhydrase and carboxyanhydrase A. Biological nitrogen fixation, Photosynthesis: Photosystem-I and Photosystem-II. Toxic metal ions and their effects, chelation therapy (examples only), Pt and Au complexes as drugs (examples only), metal dependent diseases (examples only)

### **Organometallic Chemistry**

(25 Lectures)

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands. 18-electron and 16-electron rules (pictorial MO approach). Applications of 18-electron rule to metal carbonyls, nitrosyls, cyanides. General methods of preparation of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls.  $\pi$ -acceptor behaviour of CO, synergic effect and use of IR data to explain extent of back bonding. Zeise's salt: Preparation, structure, evidences of synergic effect. Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination and insertion reactions.

### **Catalysis by Organometallic Compounds**

Study of the following industrial processes

1. Alkene hydrogenation (Wilkinson's Catalyst)
2. Hydroformylation
3. Wacker Process
4. Synthetic gasoline (Fischer Tropsch reaction)
5. Ziegler-Natta catalysis for olefin polymerization.

### Reference Books

1. Lippard, S.J. & Berg, J.M. *Principles of Bioinorganic Chemistry* Panima Publishing Company 1994.
2. 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.
3. Greenwood, N.N. & Earnshaw A. *Chemistry of the Elements*, Butterworth-Heinemann, 1997.
4. Cotton, F.A., Wilkinson, G., Murrillo, C. A., Bochmann, M., *Advanced Inorganic Chemistry 6<sup>th</sup> Ed.* 1999., Wiley.
5. Bertini, I., Gray, H. B., Lippard, S.J., Valentine, J. S., Viva, 2007.
6. Basolo, F, and Pearson, R.C. *Mechanisms of Inorganic Chemistry*, John Wiley & Sons, NY, 1967.
7. Purecell, K.F. and Kotz, J.C., *An Introduction to Inorganic Chemistry*, Saunders: Philadelphia, 1980.
8. Powell, P. *Principles of Organometallic Chemistry*, Chapman and Hall, 1988.
9. Collman, J. P. et al. *Principles and Applications of Organotransition Metal Chemistry*. Mill Valley, CA: University Science Books, 1987.
10. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*. New York, NY: John Wiley, 2000.

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## **DSE-1: ADVANCED INORGANIC CHEMISTRY (LAB)**

### **60 Lectures**

**Qualitative semimicro analysis of mixtures containing not more than three radicals. Emphasis should be given to the understanding of the chemistry of different reactions.**

Cation Radicals:  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Mn}^{2+}/\text{Mn}^{4+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Co}^{2+}/\text{Co}^{3+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Pb}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Bi}^{3+}$ ,  $\text{Sn}^{2+}/\text{Sn}^{4+}$ ,  $\text{As}^{3+}/\text{As}^{5+}$ ,  $\text{Sb}^{3+}/\text{Sb}^{5+}$ ,  $\text{NH}_4^+$ ,  $\text{Mg}^{2+}$ .

Anion Radicals:  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{BrO}_3^-$ ,  $\text{I}^-$ ,  $\text{IO}_3^-$ ,  $\text{SCN}^-$ ,  $\text{S}^{2-}$ ,  $\text{SO}_4^{2-}$ ,  $\text{NO}_3^-$ ,  $\text{NO}_2^-$ ,  $\text{PO}_4^{3-}$ ,  $\text{AsO}_4^{3-}$ ,  $\text{BO}_3^{3-}$ ,  $\text{CrO}_4^{2-} / \text{Cr}_2\text{O}_7^{2-}$ ,  $\text{Fe}(\text{CN})_6^{4-}$ ,  $\text{Fe}(\text{CN})_6^{3-}$ .

Insoluble Materials:  $\text{Al}_2\text{O}_3(\text{ig})$ ,  $\text{Fe}_2\text{O}_3(\text{ig})$ ,  $\text{Cr}_2\text{O}_3(\text{ig})$ ,  $\text{SnO}_2$ ,  $\text{SrSO}_4$ ,  $\text{BaSO}_4$ ,  $\text{CaF}_2$ ,  $\text{PbSO}_4$ .

### Reference Books

1. Svehla, G., *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
2. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015



ANY **THREE** FROM THE FOLLOWING RECOMMENDED FIVE  
(DSE-2 to DSE-7) COURSES ARE TO BE CHOSEN

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**DSE-2: ANALYTICAL METHODS IN CHEMISTRY**

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

**Optical methods of analysis: (25 Lectures)**

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.

**Thermal methods of analysis: (8 Lectures)**

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

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

**Electroanalytical methods: (12 Lectures)**

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

**Separation techniques: (15 Lectures)**

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.

### **Reference Books**

1. Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6<sup>th</sup> Ed.*, Pearson, 2009.
2. Willard, H.H. *et al.: Instrumental Methods of Analysis, 7<sup>th</sup> Ed.* Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Christian, G.D. *Analytical Chemistry, 6<sup>th</sup> Ed.* John Wiley & Sons, New York, 2004.
4. Harris, D.C.: *Exploring Chemical Analysis, 9<sup>th</sup> Ed.* New York, W.H. Freeman, 2016.
5. Khopkar, S.M. *Basic Concepts of Analytical Chemistry.* New Age International Publisher, 2009.
6. Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis,* Cengage Learning India Ed.
7. Mikes, O. *Laboratory Hand Book of Chromatographic & Allied Methods,* Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.
8. Ditts, R.V. *Analytical Chemistry; Methods of separation,* van Nostrand, 1974.

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## **PRACTICALS- DSE-2 LAB: ANALYTICAL METHODS IN**

# **CHEMISTRY**

(60 Lectures)

## **I. Separation Techniques by:**

### **Chromatography:**

(a) 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

### **Solvent Extractions:**

To separate a mixture of  $Ni^{2+}$  &  $Fe^{2+}$  by complexation with DMG and extracting the  $Ni^{2+}$ -DMG complex in chloroform, and determine its concentration by spectrophotometry.

## **II. Analysis of soil:**

- (i) Determination of pH of soil.
- (ii) Estimation of calcium, magnesium, phosphate

## **III. Ion exchange:**

Determination of exchange capacity of cation exchange resins and anion exchange resins.

## **IV. Spectrophotometry**

- 1. Determination of pKa values of indicator using spectrophotometry.
- 2. Determination of chemical oxygen demand (COD).
- 3. Determination of Biological oxygen demand (BOD).

### **Reference Books**

- 1. Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6<sup>th</sup> Ed.*, Pearson, 2009.
- 2. Willard, H.H. *et al.: Instrumental Methods of Analysis, 7<sup>th</sup> Ed.* Wardsworth Publishing Company, Belmont, California, USA, 1988.
- 3. Christian, G.D. *Analytical Chemistry, 6<sup>th</sup> Ed.* John Wiley & Sons, New York, 2004.
- 4. Harris, D.C. *Exploring Chemical Analysis, 9<sup>th</sup> Ed.* New York, W.H. Freeman, 2016.
- 5. Khopkar, S.M. *Basic Concepts of Analytical Chemistry.* New Age International Publisher, 2009.

6. Skoog, D.A. Holler F.J. and Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Edition.
  7. Mikes, O. & Chalmes, R.A. *Laboratory Handbook of Chromatographic & Allied Methods*, Elles Harwood Ltd. London.
  8. Ditts, R.V. *Analytical Chemistry: Methods of separation*. Van Nostrand, New York, 1974.
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### **DSE-3: APPLICATIONS OF COMPUTERS IN CHEMISTRY**

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

**Theory: 60 Lectures  
20)**

**(Lectures:**

**Computer Programming Basics (FORTRAN):** Elements of FORTRAN Language. FORTRAN Keywords and commands, Logical and Relational Operators, iteration, Array variables, Matrix addition and multiplication. Function and Subroutine.

**Introduction to Spreadsheet Software(MS Excel):**

**(Lectures 25)**

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.

Solution of simultaneous equations(for eg: in chemical Equilibrium problems) using Excel **SOLVER** Functions . Use of Excel Goal Seek function.

Numerical Modelling: Simulation of pH metric titration curves, Excel functions **LINEST** and Least Squares. Numerical Curve Fitting, Regression, Numerical Differentiation and Integration

**Statistical Analysis:  
20)**

**(Lectures:**

Gaussian Distribution and Errors in Measurement and their effect on data sets. Descriptive Statistics using Excel, Statistical Significance Testing, the T test and the F test.

#### **Reference Books**

1. McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
2. Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005).
3. Steiner, E. The Chemical Maths Book Oxford University Press (1996).

4. Yates, P. Chemical calculations. 2nd Ed. CRC Press (2007).
5. Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007) Chapters 3-5.
6. Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001)
7. Noggle, J. H. Physical chemistry on a Microcomputer. Little Brown & Co. (1985).
8. S. R. Crouch, F. J. Holler, Applications of MS Excel in Analytical Chemistry, Thomson, 2004.
9. V. Rajaraman, Computer Programming in FORTRAN 77, Prentice Hall, 1997
10. Martin Cwiakala, Schaum's Outline of Programming with FORTRAN 77, 1995

## **PRACTICALS-DSE-3 APPLICATIONS OF COMPUTERS IN CHEMISTRY**

### **(60 Lectures)**

( At least 10 experiments are to be performed.)

1. Plotting of Graphs using a spreadsheet. ( Planck's Distribution Law, Maxwell Boltzmann Distribution Curves as a function of temperature and molecular weight
2. Determination of vapour pressure from Van der Waals Equation of State.
3. Determination of rate constant from Concentration-time data using **LINEST** function.
4. Determination of Molar Extinction Coefficient from Absorbent's data using **LINEST** function.
5. Determination of concentration simultaneously using Excel **SOLVER** Function.(For eg: Determination of  $[\text{OH}^-]$ ,  $[\text{Mg}^{2+}]$  and  $[\text{H}_3\text{O}^+]$  from  $K_{\text{sp}}$  and  $K_{\text{w}}$  data of  $\text{Mg}(\text{OH})_2$ .)
6. Simultaneous Solution of Chemical Equilibrium Problems to determine the equilibrium compositions from the Equilibrium Constant data at given Pressure and Temperature.
7. Determination of Molar Enthalpy of Vaporization using Linear and Non Linear Least squares fit.
8. Calculation and Plotting of a Precipitation Titration Curve with MS Excel.
9. Acid-Base Titration Curve using Excel **Goal Seek** Function.
10. Plotting of First and Second Derivative Curve for pH metric and Potentiometric titrations .
11. Use of spreadsheet to solve the 1D Schrodinger Equation(Numerov Method).
12. Michaelis-Menten Kinetics for Enzyme Catalysis using Linear and Non - Linear Regression

### **Reference Books**

1. Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001)

2. S. R. Crouch, F. J. Holler, Applications of MS Excel in Analytical Chemistry, Thomson, 2004.
3. Levine, I. N. Physical Chemistry, Tata McGraw-Hill ,6th Edition

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## **DSE-4: GREEN CHEMISTRY**

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

**Theory: 60 Lectures**

**Introduction to Green Chemistry: (04 Lectures)**

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

**Principles of Green Chemistry and Designing a Chemical synthesis: (30 Lectures)**

Twelve principles of Green Chemistry with their explanations and examples and special emphasis on the following:

- 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, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
- Prevention/ minimization of hazardous/ toxic products reducing toxicity.  $\text{risk} = (\text{function}) \text{hazard} \times \text{exposure}$ ; waste or pollution prevention hierarchy.
- Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents.
- Energy requirements for reactions – alternative sources of energy: use of microwaves and 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; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.
- Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

**Examples of Green Synthesis/ Reactions and some real world cases: (16 Lectures)**

1. Green Synthesis of the following compounds: adipic acid, catechol, disodium

- iminodiacetate (alternative to Strecker synthesis)
2. Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction
  3. Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)
  4. Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments.

### **Future Trends in Green Chemistry:**

**(10 Lectures)**

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co crystal controlled solid state synthesis (C<sup>2</sup>S<sup>3</sup>); Green chemistry in sustainable development.

#### **Reference Books**

1. Anastas, P.T. & Warner, J.K.: *Green Chemistry - Theory and Practical*, Oxford University Press (1998).
2. Matlack, A.S. *Introduction to Green Chemistry*, Marcel Dekker (2001).
3. Cann, M.C. & Connely, M.E. *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).
4. Ryan, M.A. & Tinnesand, M. *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).
5. Lancaster, M. *Green Chemistry: An Introductory Text* RSC Publishing, 2<sup>nd</sup> Edition, 2010.

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## **PRACTICALS-DSE-4 LAB GREEN CHEMISTRY**

**(60 Lectures)**

### **1. Safer starting materials**

- Preparation and characterization of nanoparticles of gold using tea leaves.

### **2. Using renewable resources**

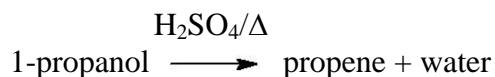
- Preparation of biodiesel from vegetable/ waste cooking oil.

### **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

Triethylamine ion + OH<sup>-</sup> → propene + trimethylpropene + water



- 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.

#### 5. Alternative Green solvents

- Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared from dry ice.

Mechanochemical solvent free synthesis of azomethines

#### 6. Alternative sources of energy

- Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).
- Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

#### Reference Books

1. Anastas, P.T & Warner, J.C. *Green Chemistry: Theory and Practice*, Oxford University Press (1998).
2. Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).
3. Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, Washington DC (2002).
4. 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).
5. Cann, M.C. & Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society (2008).
6. Cann, M. C. & Thomas, P. *Real world cases in Green Chemistry*, American Chemical Society (2008).
7. Lancaster, M. *Green Chemistry: An Introductory Text* RSC Publishing, 2<sup>nd</sup> Edition, 2010.
8. Pavia, D.L., Lampman, G.M., Kriz, G.S. & Engel, R.G. *Introduction to Organic Laboratory Techniques: A Microscale and Macro Scale Approach*, W.B.Saunders, 1995.



## **DSE - 5 INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE**

**(Credits: Theory-06, Practicals-02)  
60 Lectures**

### **Silicate Industries: (16 Lectures)**

*Glass:* Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

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

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

### **Fertilizers: (8 Lectures)**

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

### **Surface Coatings: (10 Lectures)**

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

### **Batteries: (6 Lectures)**

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

### **Alloys: (10 Lectures)**

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 (Ar and heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

**Catalysis: (6 Lectures)**

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

Phase transfer catalysts, application of zeolites as catalysts.

**Chemical explosives: (4 Lectures)**

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

**Reference Books**

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
4. J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
5. P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
6. R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
7. Sharma, B.K. & Gaur, H. *Industrial Chemistry*, Goel Publishing House, Meerut (1996).

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**PRACTICALS-DSE 5 LAB INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE**

**(60 Lectures)**

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

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
4. J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
5. P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
6. R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
7. Publications, New Delhi.
8. Sharma, B.K. & Gaur, H. *Industrial Chemistry*, Goel Publishing House, Meerut (1996).

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## **CHEMISTRY-DSE- 6: POLYMER CHEMISTRY**

(Credits: Theory-06, Practicals-02)

**Theory: 60 Lectures**

**Introduction and history of polymeric materials: (04 Lectures)**

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

**Functionality and its importance: (08 Lectures)**

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.

**Kinetics of Polymerization: (08 Lectures)**

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

**Crystallization and crystallinity: (04 Lectures)**

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

**Nature and structure of polymers: (04 Lectures)**

Structure Property relationships.

**Determination of molecular weight of polymers: (08 Lectures)**

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

**Glass transition temperature ( $T_g$ ) and determination of  $T_g$ : (08 Lectures)**

Free volume theory, WLF equation, Factors affecting glass transition temperature ( $T_g$ ).

**Polymer Solution: (08 Lectures)**

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 Polymer: (10 Lectures)**

(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)].

**Reference Books**

1. R.B. Seymour & C.E. Carraher: *Polymer Chemistry: An Introduction*, Marcel Dekker, Inc. New York, 1981.
2. G. Odian: *Principles of Polymerization*, 4<sup>th</sup> Ed. Wiley, 2004.
3. F.W. Billmeyer: *Textbook of Polymer Science*, 2<sup>nd</sup> Ed. Wiley Interscience, 1971.
4. P. Ghosh: *Polymer Science & Technology*, Tata McGraw-Hill Education, 1991.
5. R.W. Lenz: *Organic Chemistry of Synthetic High Polymers*. Interscience Publishers, New York, 1967.

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**PRACTICALS – DSE- 6 LAB: POLYMER CHEMISTRY**

**(60 Lectures)**

**Polymer synthesis**

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).
  - a) Purification of monomer
  - b) Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bis-isobutyronitrile (AIBN)

2. Preparation of nylon 66/6
3. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein
4. Redox polymerization of acrylamide
5. Precipitation polymerization of acrylonitrile
6. Preparation of urea-formaldehyde resin
7. Preparations of novalac resin/ resold resin.
8. Microscale Emulsion Polymerization of Poly(methylacrylate).

### **Polymer characterization**

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

### **Polymer analysis**

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

\*at least 7 experiments to be carried out.

### **Reference Books**

1. M.P. Stevens, *Polymer Chemistry: An Introduction*, 3<sup>rd</sup> Ed., Oxford University Press, 1999.
2. H.R. Allcock, F.W. Lampe & J.E. Mark, *Contemporary Polymer Chemistry*, 3<sup>rd</sup> ed. Prentice-Hall (2003)
3. F.W. Billmeyer, *Textbook of Polymer Science*, 3<sup>rd</sup> ed. Wiley-Interscience (1984)
4. J.R. Fried, *Polymer Science and Technology*, 2<sup>nd</sup> ed. Prentice-Hall (2003)
5. P. Munk & T.M. Aminabhavi, *Introduction to Macromolecular Science*, 2<sup>nd</sup> ed. John Wiley & Sons (2002)

6. L. H. Sperling, *Introduction to Physical Polymer Science*, 4<sup>th</sup> ed. John Wiley & Sons (2005)
7. M.P. Stevens, *Polymer Chemistry: An Introduction* 3<sup>rd</sup> ed. Oxford University Press (2005).
8. Seymour/ Carraher's *Polymer Chemistry*, 9<sup>th</sup> ed. by Charles E. Carraher, Jr. (2013).

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## ***CHEMISTRY-DSE7: MOLECULAR MODELLING & DRUG DESIGN***

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

### **Introduction to Molecular Modelling: (8 Lectures)**

Introduction. Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces.

### **Force Fields: (12 Lectures)**

Bond Stretching. Angle Bending. Introduction to nonbonded interactions. Electrostatic interactions. van der Waals Interactions. Hydrogen bonding in Molecular Mechanics. Force Field Models for the Simulation of Liquid Water.

### **Energy Minimization and Computer Simulation: (12 Lectures)**

Minimization and related methods for exploring the energy surface. Non-derivative method, First and second order minimization methods. Computer simulation methods. Simple thermodynamic properties and Phase Space. Boundaries. Analyzing the results of a simulation and estimating Errors

### **Molecular Dynamics & Monte Carlo Simulation: (16 Lectures)**

Molecular Dynamics Simulation Methods. Molecular Dynamics using simple models. Molecular Dynamics with continuous potentials. Molecular Dynamics at constant temperature and pressure. Metropolis method. Monte Carlo simulation of molecules.

### **Structure Prediction and Drug Design: (12 Lectures)**

Structure prediction - Introduction to comparative Modeling. Sequence alignment. Constructing and evaluating a comparative model. Predicting protein structures by 'Threading', Molecular docking. Structure based de novo ligand design, QSAR.

### **Reference Books:**

1. A.R. Leach, *Molecular Modelling Principles and Application*, Longman, 2001.
2. J.M. Haile, *Molecular Dynamics Simulation Elementary Methods*, John Wiley and

Sons, 1997.

3. Satya Prakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.

## ***PRACTICAL- DSE7 LAB: MOLECULAR MODELLING & DRUG DESIGN***

(60 Lectures)

- i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane  $\sigma$  bonds and ethene, ethyne, benzene and pyridine  $\pi$  bonds.
- ii. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.
- iii. Visualize the electron density and electrostatic potential maps for LiH, HF, N<sub>2</sub>, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
- iv. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- v. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- vi. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
- vii. (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- viii. Arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
- ix. (a) Compare the optimized bond angles H<sub>2</sub>O, H<sub>2</sub>S, H<sub>2</sub>Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.

*Note:* Software: ChemSketch, ArgusLab ([www.planaria-software.com](http://www.planaria-software.com)), TINKER 6.2 ([dasher.wustl.edu/ffe](http://dasher.wustl.edu/ffe)), WebLab Viewer, Hyperchem, VMD, or any similar software.

### **Reference Books:**

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

J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.

Satya Prakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.

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## SKILL ENHANCEMENT COURSES (Honours in Chemistry)

### SEC T1 – Mathematics and Statistics for Chemists

(Credits: 2 Lectures: 30)

1. Functions, limits, derivative, physical significance, basic rules of differentiation, maxima and minima, applications in chemistry, Error function, Gamma function, exact and inexact differential, Taylor and McLaurin series, Fourier series and Fourier Transform, Laplace transform, partial differentiation, rules of integration, definite and indefinite integrals.

(8L)

2. **Differential equations:** Separation of variables, homogeneous, exact, linear equations, equations of second order, series solution method.

(4L)

3. **Probability** : Permutations, combinations and theory of probability (3L)

4. Vectors, matrices and determinants Vectors, dot, cross and triple products, introduction to matrix algebra, addition and multiplication of matrices, inverse, adjoint and transpose of matrices, unit and diagonal matrices.

(4 Lectures )

5. **Qualitative and quantitative aspects of analysis:** (03 Lectures)

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.

6. **Analysis and Presentation of Data:** Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit. Basic aspects of multiple linear regression analysis. (8 Lectures)

### Reference Books

1. The Chemical Maths Book, E. Steiner, Oxford University Press (1996).
2. Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
3. Higher Engineering Mathematics, Grewal B.S., Khanna Publishers, 43rd Edition.
4. Advanced Engineering Mathematics, Kreyszig Erwin, Wiley, 10th Edition



## SEC T2 – ANALYTICAL CLINICAL BIOCHEMISTRY

(Credits: 2 Lectures:30)

### Review of Concepts from Core Course

*Carbohydrates:* Biological importance of carbohydrates, Metabolism, Cellular currency of energy (ATP), Glycolysis, Alcoholic and Lactic acid fermentations, Krebs cycle.

Isolation and characterization of polysachharides.

*Proteins:* Classification, biological importance; Primary and secondary and tertiary structures of proteins:  $\alpha$ -helix and  $\beta$ -pleated sheets, Isolation, characterization, denaturation of proteins.

*Enzymes:* Nomenclature, Characteristics (mention of Ribozymes), and Classification; Active site, Mechanism of enzyme action, Stereospecificity of enzymes, Coenzymes and cofactors, Enzyme inhibitors, Introduction to Biocatalysis: Importance in “Green Chemistry” and Chemical Industry.

*Lipids:* Classification. Biological importance of triglycerides and phosphoglycerides and cholesterol; Lipid membrane, Liposomes and their biological functions and underlying applications.

*Lipoproteins:* Properties, functions and biochemical functions of steroid hormones. Biochemistry of peptide hormones.

Structure of DNA (Watson-Crick model) and RNA, Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation, Introduction to Gene therapy.

*Enzymes:* Nomenclature, classification, effect of pH, temperature on enzyme activity, enzyme inhibition.

### Biochemistry of disease: A diagnostic approach by blood/ urine analysis.

*Blood:* Composition and functions of blood, blood coagulation. Blood collection and preservation of samples. Anaemia, Regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin.

*Urine:* Collection and preservation of samples. Formation of urine. Composition and estimation of constituents of normal and pathological urine.

### Hands On Practical

Identification and estimation of the following:

1. Carbohydrates – qualitative and quantitative.
2. Lipids – qualitative.
3. Determination of the iodine number of oil.
4. Determination of the saponification number of oil.
5. Determination of cholesterol using Liebermann- Burchard reaction.
6. Proteins – qualitative.
7. Isolation of protein.
8. Determination of protein by the Biuret reaction.
9. Determination of nucleic acids

### Reference Books

1. Cooper, T.G. Tool of Biochemistry. Wiley-Blackwell (1977).
2. Wilson, K. & Walker, J. Practical Biochemistry. Cambridge University Press (2009).
3. Varley, H., Gowenlock, A.H & Bell, M.: Practical Clinical Biochemistry, Heinemann, London (1980).
4. Devlin, T.M., Textbook of Biochemistry with Clinical Correlations, John Wiley & Sons, 2010.
5. Berg, J.M., Tymoczko, J.L. & Stryer, L. Biochemistry, W.H. Freeman, 2002.

6. Talwar, G.P. & Srivastava, M. Textbook of Biochemistry and Human Biology, 3rd Ed. PHI Learning.
7. Nelson, D.L. & Cox, M.M. Lehninger Principles of Biochemistry, W.H. Freeman, 2013.
8. O. Mikes, R.A. Chalmers: Laboratory Handbook of Chromatographic Methods, D. Van Nostrand & Co., 1961.

### **SEC T3 – PHARMACEUTICALS CHEMISTRY**

(Credits: 2 Lectures: 30)

#### **Drugs & Pharmaceuticals**

Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol, Ibuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

#### **Fermentation**

Aerobic and anaerobic fermentation. Production of (i) Ethyl alcohol and citric acid, (ii) Antibiotics; Penicillin, Cephalosporin, Chloromycetin and Streptomycin, (iii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C.

#### **Hands On Practical**

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

#### **Reference Books**

1. Patrick, G. L. Introduction to Medicinal Chemistry, Oxford University Press, UK, 2013.
2. Singh, H. & Kapoor, V.K. Medicinal and Pharmaceutical Chemistry, Vallabh Prakashan, Pitampura, New Delhi, 2012.
3. Foye, W.O., Lemke, T.L. & William, D.A.: Principles of Medicinal Chemistry, 4th ed., B. .I. Waverly Pvt. Ltd. New Delhi.

# GENERAL ELECTIVE COURSE IN CHEMISTRY

SEM-I	SEM-I I	SEM-I II	SEM-I V	SEM-V	SEM-VI
<b>Inorganic-I</b>	<b>Organic-I</b>	<b>Inorganic-II</b>	<b>Organic-II</b>	<b>Inorganic-III</b>	<b>Organic-III</b>
<b>Physical-I</b>	Analytical & Environment	<b>Physical-II</b>	Analytical & Industrial -I	<b>Physical-III</b>	Analytical & Industrial -II

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## SEMESTER-I

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### GE T1: (Credits: Theory-04, Practicals-02)

#### Theory: 60 Lectures

#### Section A: Inorganic Chemistry-I (30 Lectures)

##### Atomic Structure (10 Lectures)

Bohr's theory for hydrogen atom (simple mathematical treatment), atomic spectra of hydrogen and Bohr's model, Sommerfeld's model, quantum numbers and their significance, Pauli's exclusion principle, Hund's rule, electronic configuration of many-electron atoms, *Aufbau* principle and its limitations.

##### Chemical Periodicity (05 Lectures)

Classification of elements on the basis of electronic configuration: general characteristics of s-, p-, d- and f-block elements. Positions of hydrogen and noble gases. Atomic and ionic radii, ionization potential, electron affinity, and electronegativity; periodic and group-wise variation of above properties in respect of s- and p- block elements.

##### Acids and bases (07 Lectures)

Brönsted–Lowry concept, conjugate acids and bases, relative strengths of acids and bases, effects of substituent and solvent, differentiating and levelling solvents. Lewis acid-base concept, classification of Lewis acids and bases, Lux-Flood concept and solvent system concept. Hard and soft acids and bases ( HSAB concept), applications of HSAB process.

##### Redox reactions (08 Lectures)

Ion-electron method of balancing equation of redox reaction. Elementary idea on standard redox potentials with sign conventions, Nernst equation (without derivation). Influence of complex formation, precipitation and change of pH on redox potentials; formal potential. Feasibility of a redox titration, redox potential at the equivalence point, redox indicators.

#### Section A: Physical Chemistry-I (30 Lectures)

##### Kinetic Theory of Gases and Real gases (10 Lectures)

Concept of pressure and temperature; Collision of gas molecules; Collision diameter; Collision number and mean free path; Frequency of binary collisions (similar molecules); Nature of distribution of velocities, Maxwell's distribution of speed and kinetic energy; Average velocity, root mean square velocity and most probable velocity; Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases

Deviation of gases from ideal behavior; compressibility factor; Boyle temperature; Andrew's and Amagat's plots; van der Waals equation and its features; its derivation and application in explaining real gas behaviour; Existence of critical state, Critical constants in

terms of van der Waals constants; Law of corresponding states. Viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only)

### **Liquids (06 Lectures)**

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

### **Solids (06 Lectures)**

Forms of solids, crystal systems, unit cells, Bravais lattice types, Symmetry elements; Laws of Crystallography - Law of constancy of interfacial angles, Law of rational indices; Miller indices of different planes and interplanar distance, Bragg's law;

### **Chemical Kinetics (08 Lectures)**

Introduction of rate law, Order and molecularity; Extent of reaction; rate constants; Rates of First, second and nth order reactions and their Differential and integrated forms (with derivation); Pseudo first order reactions; Determination of order of a reaction by half half-life and differential method. Temperature dependence of rate constant; Arrhenius equation, energy of activation; Collision theory; Lindemann theory of unimolecular reaction;

### **Reference Books:**

1. Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009). □
2. Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
3. Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
4. Chugh, K.L., Agnish, S.L. *A Text Book of Physical Chemistry* Kalyani Publishers □
5. Bahl, B.S., Bahl, A., Tuli, G.D., *Essentials of Physical Chemistry* S. Chand & Co. Ltd. □
6. Palit, S. R., *Elementary Physical Chemistry* Book Syndicate Pvt. Ltd. □
7. Mandal, A. K. *Degree Physical and General Chemistry* Sarat Book House □
8. Pahari, S., *Physical Chemistry* New Central Book Agency □

### **GE P1: 60 Lectures**

#### **Section A: Inorganic Chemistry –LAB (30 Lectures)**

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  $\text{Na}_2\text{S}_2\text{O}_3$ .
6. Estimation of Fe(II) and Fe(III) in a given mixture using  $\text{K}_2\text{Cr}_2\text{O}_7$  solution.

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#### **Section B: Physical Chemistry-LAB (15x2=30 Lectures)**

(Minimum five experiments to complete)

##### **(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 liquid or a dilute 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) Study the kinetics of the following reactions**

(i) Acid hydrolysis of methyl acetate with hydrochloric acid

(ii) Compare the strengths of HCl and H<sub>2</sub>SO<sub>4</sub> by studying kinetics of hydrolysis of methyl acetate

**Reference Books:**

1. Palit, S.R., *Practical Physical Chemistry* Science Book Agency
- 2.. Mukherjee, N.G., *Selected Experiments in Physical Chemistry* J. N. Ghose & Sons
- 3.. Dutta, S.K., *Physical Chemistry Experiments* Bharati Book Stall
4. *Practical Workbook Chemistry (Honours), UGBS, Chemistry, University of Calcutta, 2015*

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**SEMESTER-II**

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**GE T2: (Credits: Theory-04, Practicals-02)**

**Theory: 60 Lectures**

**SectionA: Organic Chemistry-I (30 Lectures)**

**Fundamentals of Organic Chemistry (5 Lectures)**

*Electronic displacements:* inductive effect, resonance and hyperconjugation; cleavage of bonds: homolytic and heterolytic; structure of organic molecules on the basis of VBT; nucleophiles electrophiles; reactive intermediates: carbocations, carbanions and free radicals.

**Stereochemistry (8 Lectures)**

Different types of isomerism; geometrical and optical isomerism; concept of chirality and optical activity (up to two carbon atoms); asymmetric carbon atom; elements of symmetry (plane and centre); interconversion of Fischer and Newman representations; enantiomerism and diastereomerism, *meso* compounds; *threo* and *erythro*, D and L, *cis* and *trans* nomenclature; CIP Rules: *R/S* (upto 2 chiral carbon atoms) and *E/Z* nomenclature.

**Nucleophilic Substitution and Elimination Reactions (5 Lectures)**

*Nucleophilic substitutions:* S<sub>N</sub>1 and S<sub>N</sub>2 reactions; eliminations: E1 and E2 reactions (elementary mechanistic aspects); Saytzeff and Hofmann eliminations; elimination vs substitution.

**Aliphatic Hydrocarbons (12 Lectures)**

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

*Alkanes:* (up to 5 Carbons). *Preparation:* catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. *Reactions:* mechanism for free radical substitution: halogenation.

*Alkenes:* (up to 5 Carbons). *Preparation:* elimination reactions: dehydration of alcohols and dehydrohalogenation of alkyl halides; *cis* alkenes (partial catalytic hydrogenation) and *trans* alkenes (Birch reduction). *Reactions:* *cis*-addition (alkaline  $\text{KMnO}_4$ ) and *trans*-addition (bromine) with mechanism, addition of HX [Markownikoff's (with mechanism) and anti-Markownikoff's addition], hydration, ozonolysis, oxymercuration-demercuration and hydroboration-oxidation reaction.

*Alkynes:* (up to 5 Carbons). *Preparation:* acetylene from  $\text{CaC}_2$  and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal dihalides.

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

#### **Reference Books:**

1. Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991. □
2. Cotton, F.A., Wilkinson, G. & Gaus, P.L. *Basic Inorganic Chemistry*, 3rd ed., Wiley. □
3. Douglas, B.E., McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry*, John Wiley & Sons.
4. Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Education India, 2006. □□□□□
5. Sethi, A. *Conceptual Organic Chemistry*; New Age International Publisher.
6. Parmar, V. S. *A Text Book of Organic Chemistry*, S. Chand & Sons.
7. Madan, R. L. *Organic Chemistry*, S. Chand & Sons.

#### **Section B**

##### **GE T2 Section B: Analytical and Environmental Chemistry (30 Lectures)**

##### **Chemical Analysis (15 Lectures)**

*Gravimetric analysis:* solubility product and common ion effect; requirements of gravimetry; gravimetric estimation of chloride, sulphate, lead, barium, nickel, copper and zinc.

*Volumetric analysis:* primary and secondary standard substances; principles of acid-base, oxidation-reduction and complexometric titrations; indicators: acid-base, redox and metal ion; principles of estimation of mixtures:  $\text{NaHCO}_3$  and  $\text{Na}_2\text{CO}_3$  (by acidimetry); iron, copper, manganese and chromium (by redox titration); zinc, aluminum, calcium and magnesium (by complexometric EDTA titration).

*Chromatography:* chromatographic methods of analysis: column chromatography and thin layer chromatography.

##### **Environmental Chemistry (15 Lectures)**

*The Atmosphere:* composition and structure of the atmosphere; troposphere, stratosphere, mesosphere and thermosphere; ozone layer and its role; major air pollutants: CO,  $\text{SO}_2$ ,  $\text{NO}_x$  and particulate matters – their origin and harmful effects; problem of ozone layer depletion; green house effect; acid rain and photochemical smog; air pollution episodes: air quality standard; air pollution control measures: cyclone collector, electrostatic precipitator, catalytic converter.

*The Hydrosphere:* environmental role of water, natural water sources, water treatment for industrial, domestic and laboratory uses; water pollutants; action of soaps and detergents, phosphates, industrial effluents, agricultural runoff, domestic wastes; thermal pollution, radioactive pollution and their effects on animal and plant life; water pollution episodes: water pollution control measures : waste water treatment; chemical treatment and microbial

treatment; water quality standards: DO, BOD, COD, TDS and hardness parameters; desalination of sea water : reverse osmosis, electro dialysis.

*The Lithosphere:* water and air in soil, waste matters and pollutants in soil, waste classification, treatment and disposal; soil pollution and control measures.

**Reference Books:**

1. Banerjee, S. P. *A Text Book of Analytical Chemistry*, The New Book Stall.
2. Gangopadhyay, P. K. *Application Oriented Chemistry*, Book Syndicate.
3. Mondal, A. K & Mondal, S. *Degree Applied Chemistry*, Sreedhar Publications

**GE P2: 60 Lectures**

**Section A: Organic Chemistry- LAB (30 Lectures)**

*Qualitative Analysis of Single Solid Organic Compound(s)*

Experiment A: Detection of special elements (N, Cl, and S) in organic compounds.

Experiment B: Solubility and Classification (solvents: H<sub>2</sub>O, dil. HCl, dil. NaOH)

Experiment C: Detection of functional groups: Aromatic-NO<sub>2</sub>, Aromatic -NH<sub>2</sub>, -COOH, carbonyl (no distinction of -CHO and >C=O needed), -OH (phenolic) in solid organic compounds.

Experiments A - C with unknown (at least 6) solid samples containing not more than two of the above type of functional groups should be done.

**Reference Books:**

1. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015
2. Das, S. C., Chakraborty, S. B., *Practical Chemistry*.
3. Mukherjee, K. S. *Text book on Practical Chemistry*, New Oriental Book Agency.
4. Ghosal, Mahapatra & Nad, *An Advanced course in practical Chemistry*, New Central Book Agency.
5. Vogel, A. I. *Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis*, CBS Publishers and Distributors.
6. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
7. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.

**Section B: Analytic and Environmental Chemistry-LAB (30 Lectures)**

1. To find the total hardness of water by EDTA titration.
2. To find the PH of an unknown solution by comparing color of a series of HCl solutions + 1 drop of methyl orange, and a similar series of NaOH solutions + 1 drop of phenolphthalein.
3. To determine the rate constant for the decomposition of Hydrogen Peroxide
4. Determination of the strength of the H<sub>2</sub>O<sub>2</sub> sample.
5. To determine the solubility of a sparingly soluble salt, e.g. KHTa (one bottle)

**Reference Books:**

1. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011). □
2. Ghosal, Mahapatra & Nad, *An Advanced Course in Practical Chemistry*, New Central

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## SEMESTER-III

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### GE T3:

#### *Inorganic Chemistry-II (30 Lectures)*

##### **Chemical Bonding and Molecular Structure (16 Lectures)**

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

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

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

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

##### **Comparative study of p-block elements: (14 Lectures)**

Group trends in electronic configuration, modification of pure elements, common oxidation states, inert pair effect, and their important compounds in respect of the following groups of elements:

- i) B-Al-Ga-In-Tl
- ii) C-Si-Ge-Sn-Pb
- iii) N-P-As-Sb-Bi
- iv) O-S-Se-Te
- v) F-Cl-Br-I

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

1. Cotton, F.A. & Wilkinson, G. *Basic Inorganic Chemistry*, Wiley. □
2. Shriver, D.F. & Atkins, P.W. *Inorganic Chemistry*, Oxford University Press.
3. Wulfsberg, G. *Inorganic Chemistry*, Viva Books Pvt. Ltd. □
4. Rodgers, G.E. *Inorganic & Solid State Chemistry*, Cengage Learning India Ltd., 2008. □

##### **SectionB: Physical Chemistry-II (30 Lectures)**

##### **Chemical Energetics (14 Lectures)**

Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics; Concept of heat, work, internal energy and statement of first law; enthalpy, H; relation between heat capacities, calculations of q, w, U and H for reversible, irreversible and free expansion of gases.

Standard states; Heats of reaction; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; Laws of thermochemistry; bond energy, bond dissociation energy and resonance energy from thermochemical data, Kirchhoff's equations and effect of pressure on enthalpy of reactions; Adiabatic flame temperature; explosion temperature.



Statement of the second law of thermodynamics; Concept of heat reservoirs and heat engines; Carnot cycle; Physical concept of Entropy; Carnot engine, refrigerator and efficiency; Entropy change of systems and surroundings for various processes and transformations; Auxiliary state functions (G and A) and Criteria for spontaneity and equilibrium.

**Chemical Equilibrium: (08 Lectures)**

Thermodynamic conditions for equilibrium, degree of advancement; Variation of free energy with degree of advancement; Equilibrium constant and standard Gibbs free energy change; Definitions of  $K_P$ ,  $K_C$  and  $K_x$  and relation among them; van't Hoff's reaction isotherm, isobar and isochore from different standard states; Shifting of equilibrium due to change in external parameters e.g. temperature and pressure; variation of equilibrium constant with addition to inert gas; Le Chatelier's principle

**Ionic Equilibria: (08 Lectures)**

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

**Reference Books:**

1. Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009). □
2. Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
3. Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
4. Chugh, K.L., Agnish, S.L. *A Text Book of Physical Chemistry* Kalyani Publishers □
5. Bahl, B.S., Bahl, A., Tuli, G.D., *Essentials of Physical Chemistry* S. Chand & Co. Ltd. □
6. Palit, S. R., *Elementary Physical Chemistry* Book Syndicate Pvt. Ltd. □
7. Mandal, A. K. *Degree Physical and General Chemistry* Sarat Book House □
8. Pahari, S., *Physical Chemistry* New Central Book Agency □

**GE P3: 60 Lectures**

**Section A: Inorganic Chemistry –LAB (30 Lectures)**

**Qualitative semimicro analysis of mixtures containing two radicals. Emphasis should be given to the understanding of the chemistry of different reactions.**

Cation Radicals:  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Mn}^{2+}/\text{Mn}^{4+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Co}^{2+}/\text{Co}^{3+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Pb}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Bi}^{3+}$ ,  $\text{Sn}^{2+}/\text{Sn}^{4+}$ ,  $\text{NH}_4^+$ ,  $\text{Mg}^{2+}$ .

Anion Radicals:  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{BrO}_3^-$ ,  $\text{I}^-$ ,  $\text{IO}_3^-$ ,  $\text{SCN}^-$ ,  $\text{S}^{2-}$ ,  $\text{SO}_4^{2-}$ ,  $\text{NO}_3^-$ ,  $\text{NO}_2^-$ ,  $\text{PO}_4^{3-}$ ,  $\text{AsO}_4^{3-}$ ,  $\text{BO}_3^{3-}$ ,  $\text{CrO}_4^{2-} / \text{Cr}_2\text{O}_7^{2-}$

**Reference Books:**

1. Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012. □
2. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
3. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015

## **Section B: Physical Chemistry-LAB (30 Lectures)**

### **Ionic Equilibria**

- 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 and compare it with the indicator method
- b) Preparation of buffer solutions and find the pH of an unknown buffer solution by colour matching method (using following buffers)
- (i) Sodium acetate-acetic acid
- (ii) Ammonium chloride-ammonium hydroxide

### **Conductometric Titration:**

- a) Titration of a strong acid by a strong base
- b) Titration of a weak acid by a strong base

### **Reference Books:**

1. Palit, S.R., *Practical Physical Chemistry* Science Book Agency
- 2.. Mukherjee, N.G., *Selected Experiments in Physical Chemistry* J. N. Ghose & Sons
- 3.. Dutta, S.K., *Physical Chemistry Experiments* Bharati Book Stall
4. *Practical Workbook Chemistry (Honours), UGBS, Chemistry, University of Calcutta, 2015*

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## **SEMESTER-IV**

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### **GE T 4:**

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

**Theory: 60 Lectures**

### **Section-A: Organic Chemistry-II (30 Lectures)**

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

#### **Aromatic Hydrocarbons 06 Lectures)**

*Benzene: Preparation:* from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. *Reactions:* electrophilic substitution (general mechanism); nitration (with mechanism), halogenations (chlorination and bromination), sulphonation and Friedel-Craft's reaction (alkylation and acylation) (up to 4 carbons on benzene); side chain oxidation of alkyl benzenes (up to 4 carbons on benzene).

#### **Organometallic Compounds (2 Lectures)**

Introduction; *Grignard reagents: Preparations* (from alkyl and aryl halide); concept of *umpolung*; Reformatsky reaction.

#### **Aryl Halides (3 Lectures)**

*Preparation:* (chloro-, bromo- and iodobenzene): from phenol, Sandmeyer reactions. *Reactions (Chlorobenzene):* nucleophilic aromatic substitution (replacement by -OH group) and effect of nitro substituent (activated nucleophilic substitution).

### **Alcohols, Phenols and Ethers (11 Lectures)**

*Alcohols:* (up to 5 Carbons). *Preparation:* 1°-, 2°- and 3°- alcohols: using Grignard reagent, reduction of aldehydes, ketones, carboxylic acid and esters; *Reactions:* With sodium, HX (Lucas test), oxidation (alkaline KMnO<sub>4</sub>, acidic dichromate, concentrated HNO<sub>3</sub>); Oppenauer oxidation;

*Diols:* *Preparation* (with OsO<sub>4</sub>); pinacol- pinacolone rearrangement (with mechanism) (with symmetrical diols only).

*Phenols:* *Preparation:* cumene hydroperoxide method, from diazonium salts; acidic nature of phenols; *Reactions:* electrophilic substitution: nitration and halogenations; Reimer - Tiemann reaction, Houben-Hoesch condensation, Schotten -Baumann reaction, Fries rearrangement and Claisen rearrangement.

*Ethers:* *Preparation:* Williamson's ether synthesis; *Reaction:* cleavage of ethers with HI.

### **Carbonyl Compounds (08 Lectures)**

*Aldehydes and Ketones (aliphatic and aromatic):* (Formaldehyde, acetaldehyde, acetone and benzaldehyde): *Preparation:* from acid chlorides, from nitriles and from Grignard reagents; general properties of aldehydes and ketones; *Reactions:* with HCN, ROH, NaHSO<sub>3</sub>, NH<sub>2</sub>-G derivatives and with Tollens' and Fehling's reagents; iodoform test; aldol condensation (with mechanism); Cannizzaro reaction (with mechanism), Wittig reaction, benzoin condensation; Clemmensen reduction, Wolff- Kishner reduction and Meerwein-Ponndorf-Verley (MPV) reduction.

#### **Reference Books:**

1. Sethi, A. *Conceptual Organic Chemistry*; New Age International Publisher.
2. Parmar, V. S. *A Text Book of Organic Chemistry*, S. Chand & Sons.
3. Madan, R. L. *Organic Chemistry*, S. Chand & Sons.
4. Wade, L. G., Singh, M. S., *Organic Chemistry*, Pearson.
5. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
6. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
7. Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.

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### **Section-B: Analytical and Industrial Chemistry-I (30 Lectures)**

#### **Error Analysis and Computer Applications (15 Lectures)**

*Error analysis:* accuracy and precision of quantitative analysis, determinate, indeterminate, systematic and random errors; methods of least squares and standard deviations.

*Computer applications:* general introduction to computers, different components of a computer; hardware and software; input and output devices; binary numbers and arithmetic; introduction to computer languages; programming and operating

#### **Industrial Chemistry I (15 Lectures)**

*Fuels:* classification of fuel; heating values; origin of coal, carbonization of coal, coal gas, producer gas, water gas, coal based chemicals; origin and composition of petroleum, petroleum refining, cracking, knocking, octane number, antiknock compounds, kerosene, liquefied petroleum gas (LPG), liquefied natural gas (LNG); petrochemicals (C1 to C3 compounds and their uses).

*Fertilizers:* manufacture of ammonia and ammonium salts, urea, superphosphate, biofertilizers.

*Glass and ceramics:* definition and manufacture of glasses, optical glass and coloured glass; clay and feldspar, glazing and vitrification, glazed porcelain, enamel.

*Cement:* portland cement: composition and setting of cement, white cement.

**Reference Books:**

1. Cotton, F.A. & Wilkinson, G. *Basic Inorganic Chemistry*, Wiley. □
2. Shriver, D.F. & Atkins, P.W. *Inorganic Chemistry*, Oxford University Press. □
3. Wulfsberg, G. *Inorganic Chemistry*, Viva Books Pvt. Ltd. □
4. Rodgers, G.E. *Inorganic & Solid State Chemistry*, Cengage Learning India Ltd., 2008. □
5. Gangopadhyay, P. K. *Application Oriented Chemistry*, Book Syndicate. □
6. Mondal, A. K & Mondal, S. *Degree Applied Chemistry*, Sreedhar Publications. □
7. Banerjee, S. P. *A Text Book of Analytical Chemistry*, The New Book Stall □

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**GE P4: 60 Lectures**

**Section B: Organic Chemistry-LAB (30 Lectures)**

**1. Separation** based upon solubility, by using common laboratory reagents like water (cold, hot), dil. HCl, dil. NaOH, dil. NaHCO<sub>3</sub>, etc., of components of a binary solid mixture; purification of **any one** of the separated components by crystallization and determination of its melting point. The composition of the mixture may be of the following types [**ANY THREE**]: *p*-Nitrobenzoic acid/*p*-Aminobenzoic acid; *p*-Nitrotoluene/*p*-Anisidine; benzoic acid/ naphthalene; urea/phenyl-benzoate; *p*-toluidine/benzophenone; *p*-chlorobenzoic acid/ benzophenone; etc. USE of pH PAPER is recommended.

**2. Identification of a pure organic compound**

*Solid compounds:* oxalic acid, tartaric acid, succinic acid, resorcinol, urea, glucose, benzoic acid and salicylic acid.

*Liquid Compounds:* methyl alcohol, ethyl alcohol, acetone, aniline, dimethylaniline, benzaldehyde, chloroform and nitrobenzene

**Reference Books:**

1. Bhattacharyya, R. C, *A Manual of Practical Chemistry*.
2. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
3. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960. □

**Section B: Analytic Chemistry-LAB (30 Lectures)**

**I. Separation Techniques**

**Chromatography:**

**Separation of mixtures**

(a) Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the R<sub>f</sub> 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

## 2. Solvent Extractions:

To separate a mixture of  $Ni^{2+}$  &  $Fe^{2+}$  by complexation with DMG and extracting the  $Ni^{2+}$ -DMG complex in chloroform, and determine its concentration by spectrophotometry.

### Reference Books:

1. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015
2. Das, S. C., Chakraborty, S. B., *Practical Chemistry*.
3. Mukherjee, K. S. *Text book on Practical Chemistry*, New Oriental Book Agency.
4. Ghosal, Mahapatra & Nad, *An Advanced course in practical Chemistry*, New Central Book Agency.
5. Vogel, A. I. *Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis*, CBS Publishers and Distributors.

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## SEMESTER-V

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### GE T5:

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

### Section A: Inorganic Chemistry-III (30 Lectures)

#### Transition Elements (3d series) (12 Lectures)

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

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

#### Coordination Chemistry (08 Lectures)

Werner's coordination theory, Valence Bond Theory (VBT): Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Structural and stereoisomerism in complexes with coordination numbers 4 and 6. Drawbacks of VBT. IUPAC system of nomenclature.

#### Crystal Field Theory (10 Lectures)

Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors affecting the magnitude of D. Spectrochemical series. Comparison of CFSE for  $O_h$  and  $T_d$  complexes, Tetragonal distortion of octahedral geometry.

Jahn-Teller distortion, Square planar coordination.

### Reference Books:

1. Cotton, F.A. & Wilkinson, G. *Basic Inorganic Chemistry*, Wiley. □

2. Shriver, D.F. & Atkins, P.W. *Inorganic Chemistry*, Oxford University Press.
3. Wulfsberg, G. *Inorganic Chemistry*, Viva Books Pvt. Ltd. □
4. Rodgers, G.E. *Inorganic & Solid State Chemistry*, Cengage Learning India Ltd., 2008. □

**Section B: Physical Chemistry-III (30 Lectures)**

**Solutions (06 Lectures)**

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

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

**Phase Equilibria (08 Lectures)**

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)

**Conductance (08 Lectures)**

Conductance, cell constant, specific conductance and molar conductance; Variation of specific and equivalent conductance with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions; Equivalent and molar conductance at infinite dilution and their determination for strong and weak electrolytes; Ostwald's dilution law; Application of conductance measurement (determination of solubility product and ionic product of water); Conductometric titrations (acid-base)

Transport Number and principles of Hittorf's and Moving-boundary method

**Electromotive force (08 Lectures)**

Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry; Chemical cells, reversible and irreversible cells with examples; Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential; Electrochemical series; Thermodynamics of a reversible cell, calculation of thermodynamic properties:  $G$ ,  $H$  and  $S$  from EMF data

Concentration cells with and without transference, liquid junction potential; pH determination using hydrogen electrode and quinhydrone; Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation)

**Reference Books:**

1. Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009). □
2. Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
3. Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
4. Chugh, K.L., Agnish, S.L. *A Text Book of Physical Chemistry* Kalyani Publishers □
5. Bahl, B.S., Bahl, A., Tuli, G.D., *Essentials of Physical Chemistry* S. Chand & Co. Ltd. □
6. Palit, S. R., *Elementary Physical Chemistry* Book Syndicate Pvt. Ltd. □
7. Mandal, A. K. *Degree Physical and General Chemistry* Sarat Book House □
8. Pahari, S., *Physical Chemistry* New Central Book Agency □

## GE P5: 60 Lectures

### Section A: Inorganic Chemistry-III (LAB) (30 Lectures)

Gravimetric and Complexometric estimation of metals ions:

1. Estimate the amount of nickel present in a given solution as bis(dimethylglyoximate) nickel(II) or aluminium as oxine in a given solution gravimetrically.
2. Estimation of (i)  $Mg^{2+}$  or (ii)  $Zn^{2+}$  by complexometric titrations using EDTA.

Preparation of any two of the following complexes and measurement of their conductivity:

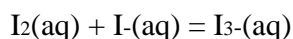
- a. tetraamminecarbonatocobalt (III) nitrate
- b. tetraamminecopper (II) sulphate
- c. potassium trioxalatoferrate (III) trihydrate

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

### Section B: Physical Chemistry-LAB (15x2=30 Lectures)

(I) Distribution Law

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



(II) Conductance

a) Determination of dissociation constant of a weak acid (cell constant, equivalent conductance are also determined)

b) Perform the following conductometric titrations: (Any **one**)

- (i) Strong acid vs. strong base
- (ii) Weak acid vs. strong base

(IV) Potentiometry

Perform the following potentiometric titrations:

- (i) Potassium Permanganate vs. Mohr's salt
- (ii) Potassium dichromate vs. Mohr's salt

### Reference Books:

1. Palit, S.R., *Practical Physical Chemistry* Science Book Agency
2. Mukherjee, N.G., *Selected Experiments in Physical Chemistry* J. N. Ghose & Sons
3. Dutta, S.K., *Physical Chemistry Experiments* Bharati Book Stall
4. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015

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## SEMESTER-VI

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### GE T6 (Credits: Theory-04, Practicals-02)

#### Theory: 30 Lectures

##### Section A: Organic Chemistry-III (30 Lectures)

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

##### Carboxylic Acids and Their Derivatives (10 Lectures)

*Carboxylic acids* (aliphatic and aromatic): strength of organic acids: comparative study with emphasis on factors affecting pK values; *Preparation*: acidic and alkaline hydrolysis of esters ( $B_{Ac2}$  and  $A_{Ac2}$  mechanisms only) and from Grignard reagents; *Reactions*: Hell - Vohlard - Zelinsky reaction and Claisen condensation; Perkin reaction.

*Carboxylic acid derivatives* (aliphatic): (up to 5 carbons). *Preparation*: acid chlorides, anhydrides, esters and amides from acids; *Reactions*: Comparative study of nucleophilicity of acyl derivatives; interconversion among acid derivatives.

##### Amines and Diazonium Salts (10 Lectures)

*Amines* (aliphatic and aromatic): strength of organic bases; *Preparation*: from alkyl halides, Gabriel's phthalimide synthesis, Hofmann degradation, by reduction of nitro compounds; *Reactions*: with  $HNO_2$  (distinction of 1 $^\circ$ -, 2 $^\circ$ - and 3 $^\circ$ - amines), Schotten - Baumann reaction, Diazo coupling reaction (with mechanism).

*Diazonium salts*: *Preparation*: from aromatic amines; *Reactions*: conversion to benzene, phenol, benzoic acid and nitrobenzene.

*Nitro compounds* (aromatic): reduction under different conditions (acidic, neutral and alkaline).

##### Amino Acids and Carbohydrates (10 Lectures)

*Amino Acids*: *Preparations* (glycine and alanine only): Strecker synthesis, Gabriel's phthalimide synthesis; general properties; zwitterion, isoelectric point; ninhydrin reaction.

*Carbohydrates*: classification and general properties; glucose and fructose: constitution; osazone formation; oxidation-reduction reactions; epimers of glucose (definition and example only); cyclic structures of glucose (determination of ring-size excluded); ascending (Kiliani -Fischer method) and descending (Ruff's and Wohl's methods) in monosaccharides (aldoses only); mutarotation.

##### Section-B: Analytical and Industrial Chemistry-II (30 Lectures)

*Polymers*: basic concept, structure and types of plastics, polythene, polystyrene, phenol-formaldehydes, PVC; manufacture, physical properties and uses of natural rubber, synthetic rubber, silicone rubber; synthetic fibres, nylon-66, polyester, terylene, rayon; foaming agents, plasticizers and stabilizers.

*Paints*: primary constituents; formulation of paints; binders and solvents for paints; oil based paints, latex paints, alkyd resin paint.

*Varnishes*: constituents of varnishes; formulation of varnishes.

*Synthetic dyes*: synthesis of methyl orange, congo red, malachite green, crystal violet.

*Drugs and pharmaceuticals*: concept and necessity of drugs and pharmaceuticals; preparation and uses: aspirin, paracetamol, sulphadiazine, quinine, chloroquine, phenobarbital, metronidazole.

*Fermentation chemicals*: production and purification of ethyl alcohol, citric acid, lactic acid, vitamin B<sub>12</sub>, penicillin.



*Fats and oils*: natural fat, edible and inedible oil of vegetable origin; common fatty acids; glycerides; hydrogenation of unsaturated oil, production of vanaspati and margarine.

*Soaps and detergents*: production of toilet and washing soaps; enzyme-based detergents, detergent powder; liquid soaps.

*Pesticides*: common pesticides: production, applications and residual toxicity of gamma-hexachlorocyclohexane, aldrin, parathion, malathion, DDT, paraquat, decamethrin.

*Food additives*: food flavour, food colour, food preservatives, artificial sweeteners, acidulants, alkalies, edible emulsifiers and edible foaming agents, sequesterants – uses and abuses of these substances in food beverages.

#### **Reference Books:**

1. Sethi, A. *Conceptual Organic Chemistry*; New Age International Publisher.
2. Parmar, V. S. A Text Book of *Organic Chemistry*, S. Chand & Sons.
3. Madan, R. L. *Organic Chemistry*, S. Chand & Sons.
4. Ekambaram, S. *General Chemistry*, Pearson.
5. Wade, L. G., Singh, M. S., *Organic Chemistry*.
6. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd.(Pearson Education).
7. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt.Ltd. (Pearson Education).
8. Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.
9. Gangopadhyay, P. K. *Application Oriented Chemistry*, Book Syndicate.
10. Mondal, A. K & Mondal, S. *Degree Applied Chemistry*, Sreedhar Publications.
11. Banerjee, S. P. *A Text Book of Analytical Chemistry*, The New Book Stall.

### **GE P6: FUNCTIONAL GROUP ORGANIC CHEMISTRY AND INDUSTRIAL CHEMISTRY LAB**

#### **30 Lectures**

#### **Section A: Organic Chemistry-III (LAB)**

A. The following reactions are to be performed, noting the yield of the crude product:

1. Nitration of aromatic compounds
2. Condensation reactions
3. Hydrolysis of amides/imides
4. Acetylation of aromatic amines
5. Benzoylation of aromatic amines

B. Purification of the crude product is to be made by crystallisation from water / alcohol.

#### **Section B: Industrial Chemistry (LAB)**

#### **Experiments**

1. Estimation of saponification value of oil / ester / fat.
2. Estimation of available chlorine in bleaching powder.
3. Estimation of acetic acid in commercial vinegar.
4. Estimation of amino acid by formol titration.

#### **Reference Books**

1. Vogel, A. I. *Elementary Practical Organic Chemistry*, Part 1: *Small scale Preparations*, CBS Publishers and Distributors.
2. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson education.
3. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.* Pearson (2012).

4. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
5. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015.
6. Arthur, I. V. *Quantitative Organic Analysis*, Pearson.
7. Das, S. C., Chakraborty, S. B., *Practical Chemistry*.
8. Ghosal, Mahapatra & Nad, *An Advanced Course in Practical Chemistry*, New Central Book Agency

## Scheme for CBCS Curriculum for BSc. Chemistry

### Credit Distribution across Courses

Course Type	Credits		
	Total Papers	Theory + Practical	Theory*+Tutorials
Core Courses (four courses from each of the three disciplines of choice)	12	12*4 =48 12*2 =24	12*5 =60 12*1=12
Elective Courses (Two papers from each discipline of choice including paper of interdisciplinary nature)	6	6*4=24 6*2=12	6*5=30 6*1=6
Ability Enhancement Compulsory Courses	2	2*2=4	2*2=4
Skill Enhancement Courses (Skill Based)	4	4*2=8	4*2=8
<b>Totals</b>	<b>24</b>	<b>120</b>	<b>120</b>

\*Tutorials of 1 Credit will be conducted in case there is no practical component