



UNIVERSITY OF CALCUTTA

Notification No. CSR/ 12 /18

It is notified for information of all concerned that the Syndicate in its meeting held on 28.05.2018 (vide Item No.14) approved the Syllabi of different subjects in Undergraduate Honours / General / Major courses of studies (CBCS) under this University, as laid down in the accompanying pamphlet:

List of the subjects

Sl. No.	Subject	Sl. No.	Subject
1	Anthropology (Honours / General)	29	Mathematics (Honours / General)
2	Arabic (Honours / General)	30	Microbiology (Honours / General)
3	Persian (Honours / General)	31	Mol. Biology (General)
4	Bengali (Honours / General /LCC2 /AECC1)	32	Philosophy (Honours / General)
5	Bio-Chemistry (Honours / General)	33	Physical Education (General)
6	Botany (Honours / General)	34	Physics (Honours / General)
7	Chemistry (Honours / General)	35	Physiology (Honours / General)
8	Computer Science (Honours / General)	36	Political Science (Honours / General)
9	Defence Studies (General)	37	Psychology (Honours / General)
10	Economics (Honours / General)	38	Sanskrit (Honours / General)
11	Education (Honours / General)	39	Social Science (General)
12	Electronics (Honours / General)	40	Sociology (Honours / General)
13	English ((Honours / General/ LCC1/ LCC2/AECC1)	41	Statistics (Honours / General)
14	Environmental Science (Honours / General)	42	Urdu (Honours / General /LCC2 /AECC1)
15	Environmental Studies (AECC2)	43	Women Studies (General)
16	Film Studies (General)	44	Zoology (Honours / General)
17	Food Nutrition (Honours / General)	45	Industrial Fish and Fisheries – IFFV (Major)
18	French (General)	46	Sericulture – SRTV (Major)
19	Geography (Honours / General)	47	Computer Applications – CMAV (Major)
20	Geology (Honours / General)	48	Tourism and Travel Management – TTMV (Major)
21	Hindi (Honours / General /LCC2 /AECC1)	49	Advertising Sales Promotion and Sales Management –ASPV (Major)
22	History (Honours / General)	50	Communicative English –CMEV (Major)
23	Islamic History Culture (Honours / General)	51	Clinical Nutrition and Dietetics CNDV (Major)
24	Home Science Extension Education (General)	52	Bachelor of Business Administration (BBA) (Honours)
25	House Hold Art (General)	53	Bachelor of Fashion and Apparel Design – (B.F.A.D.) (Honours)
26	Human Development (Honours / General)	54	Bachelor of Fine Art (B.F.A.) (Honours)
27	Human Rights (General)	55	B. Music (Honours / General) and Music (General)
28	Journalism and Mass Communication (Honours / General)		

The above shall be effective from the academic session 2018-2019.

SENATE HOUSE
KOLKATA-700073
The 4th June, 2018

Paul
4/6/18
(Dr. Santanu Paul)
Deputy Registrar

COURSE CURRICULUM UNDER CHOICE BASED CREDIT SYSTEM

SYLLABUS

FOR

**BACHELOR
IN CHEMISTRY (HONOURS)**



UNIVERSITY OF CALCUTTA

Course Structure

Course Credits

Theory+ Practical

Core Course (CC)

Theory (14 Papers of 4 credits each) $14 \times 4 = 56$

Practical (14 Papers of 2 credits each) $14 \times 2 = 28$

Discipline Specific Elective Course* (DSE)

Theory (4 Papers of 4 credits each) $4 \times 4 = 16$

Practical (4 Papers of 2 credits each) $4 \times 2 = 8$

Generic Elective (GE)

Theory (4 Papers of 4 credits each) $4 \times 4 = 16$

Practical (4 Papers of 2 credits each) $4 \times 2 = 8$

Ability Enhancement Compulsory Course (AECC)

(2 Papers of 2 credits each) $2 \times 2 = 4$

Environmental Science

English/MIL Communication

Skill Enhancement Elective Course (SEC)

(2 Papers of 2 credits each) $2 \times 2 = 4$

Total credit **140**

***Optional Dissertation or project work in place of one**

Discipline Specific Elective paper (6 credits) in 6th Semester

CORE COURSES FOR B. SC. HONOURS (CHEMISTRY)

SEM	CODE*	PAPER	BRIEF DESCRIPTION
1	CEMA-CC-1-1-TH	INORGANIC CHEMISTRY-1 ORGANIC CHEMISTRY -1A	Acid-base and redox reactions Basics of Organic Chemistry
	CEMA-CC-1-1- P	PRACTICALS**	
	CEMA-CC-1-2-TH	PHYSICAL CHEMISTRY-1 ORGANIC CHEMISTRY -1B	Kinetic theory, Chemical kinetics Stereochemistry
	CEMA-CC-1-2-P	PRACTICALS	
2	CEMA-CC-2-3-TH	ORGANIC CHEMISTRY -2	Reaction Mechanism
	CEMA-CC-2-3-P	PRACTICALS	
	CEMA-CC-2-4-TH	INORGANIC CHEMISTRY-2	Chemical Bonding
	CEMA-CC-2-4-P	PRACTICALS	
3	CEMA-CC-3-5-TH	PHYSICAL CHEMISTRY-2	Chemical Thermodynamics
	CEMA-CC-3-5-P	PRACTICALS	
	CEMA-CC-3-6-TH	INORGANIC CHEMISTRY-3	s and p Block Elements
	CEMA-CC-3-6-P	PRACTICALS	
4	CEMA-CC-3-7-TH	ORGANIC CHEMISTRY -3	Alkenes, Alkynes, Carbonyls
	CEMA-CC-3-7-P	PRACTICALS	
	CEMA-CC-4-8-TH	ORGANIC CHEMISTRY - 4	Organic Synthesis, Spectroscopy
	CEMA-CC-4-8-P	PRACTICALS	
5	CEMA-CC-4-9-TH	PHYSICAL CHEMISTRY- 3	Applications of Thermodynamics, Quantum Mechanics
	CEMA-CC-4-9-P	PRACTICALS	
	CEMA-CC-4-10-TH	INORGANIC CHEMISTRY-4	Coordination Chemistry, d & f elements
	CEMA-CC-4-10-P	PRACTICALS	
6	CEMA-CC-5-11-TH	PHYSICAL CHEMISTRY -4	Quantum Chemistry, Statistical Thermodynamics
	CEMA-CC-5-11-P	PRACTICALS	
	CEMA-CC-5-12-TH	ORGANIC CHEMISTRY -5	Cyclic Compounds, Biomolecules
	CEMA-CC-5-12-P	PRACTICALS	
6	CEMA-CC-6-13-TH	INORGANIC CHEMISTRY-5	Bioinorganic and Organometallic Chemistry
	CEMA-CC-6-13-P	PRACTICALS	
	CEMA-CC-6-14-TH	PHYSICAL CHEMISTRY -5	Molecular Spectroscopy, Photochemistry
	CEMA-CC-6-14-P	PRACTICALS	

* The Course code indicates subject-type of course-semester number-paper number-theory /practical [e.g. CEMA-CC-1-1-TH/P stands for Chemistry HonoursCore Course- First Semester- Paper 1- Theoretical /Practical]

** Practicals are based on the corresponding theoretical papers.

Discipline Specific Courses (DSE)
For Semester 5

Any One from the following

DSE-A1: MOLECULAR MODELLING & DRUG DESIGN

DSE-A2: APPLICATIONS OF COMPUTERS IN CHEMISTRY

Any One from the following

DSE-B1: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE

DSE-B2: NOVEL INORGANIC SOLIDS

For Semester 6

Any One from the following

DSE-A3: GREEN CHEMISTRY AND CHEMISTRY OF NATURAL PRODUCTS

DSE-A4: ANALYTICAL METHODS IN CHEMISTRY

Any One from the following

DSE-B3: POLYMER CHEMISTRY

DSE-B4: DISSERTATION

SKILL ENHANCEMENT COURSES (SEC)

SEC-A For Semester 3 [Any one]

SEC 1 – MATHEMATICS AND STATISTICS FOR CHEMISTS
SEC 2 – ANALYTICAL CLINICAL BIOCHEMISTRY

SEC-B For Semester 4 [Any one]

SEC 3 – PHARMACEUTICALS CHEMISTRY
SEC4 - PESTICIDE CHEMISTRY

Important Guidelines

- **General Electives (GE) are to be taken preferably from Physics and Mathematics disciplines.**
- **All graphs for Physical / Inorganic Courses must be done using standard Spreadsheet Software**
- **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.

- **Each lecture is of 1 hr duration for both theory and practical classes.**
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CORE COURSES (HONOURS) IN CHEMISTRY[CEM-A]

SEMESTER-1

CEMA-CC-1-1-TH :

(Credits: Theory-04, Practicals-02)

INORGANIC CHEMISTRY-1

Theory: 40 Lectures

Extra nuclear Structure of atom

(14 Lectures)

Quantum numbers and their significance, Schrödinger's wave equation, significance of ψ and ψ^2 . 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.

Acid-Base reactions

(12 Lectures)

Acid-Base concept: Arrhenius concept, theory of solvent system (in H₂O, NH₃, SO₂ 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

(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).

Electroanalytical methods: Basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pK_a values

Solubility and solubility effect – 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*, 5th 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*, 5th Ed., Oxford University Press (2010).
5. Cotton, F.A., Wilkinson, G. and Gaus, P.L., *Basic Inorganic Chemistry* 3rd Ed.; Wiley India.
6. Sharpe, A.G., *Inorganic Chemistry*, 4th Indian Reprint (Pearson Education) 2005.
7. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity* 4th 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).

ORGANIC CHEMISTRY-1A

Theory: 20 Lectures

Basics of Organic Chemistry

Bonding and Physical Properties

(18 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 σ , σ^* , π , π^* , n – MOs; concept of HOMO, LUMO and SOMO; sketch and energy levels of π 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 [8] annulene (including mononuclear heterocyclic compounds up to 6-membered ring); concept of antiaromaticity and homoaromaticity; non-aromatic molecules; Frost diagram (qualitative drawing).

Physical properties: influence of hybridization on bond properties: bond dissociation energy (BDE) and bond energy; bond distances, bond angles; concept of bond angle strain; 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 and heat of combustion data.

General Treatment of Reaction Mechanism I

(02 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).

Reference Books

1. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
4. Carey, F. A., Giuliano, R. M. *Organic Chemistry*, Eighth edition, McGraw Hill Education, 2012.

CEMA-CC-1-1-P (45 Lectures)

**** During examination marks of the experiments will be set in 2:1 ratio for Inorganic and Organic experiments respectively.**

1) INORGANIC CHEMISTRY: I (1) LAB

(30 Lectures)

Acid and Base Titrations: (DEMO ONLY)

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 KMnO_4 solution
2. Estimation of oxalic acid OR 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 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 $K_2Cr_2O_7$.

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

2) **ORGANIC CHEMISTRY: O (1A) LAB** (15 Lectures)

Separation based upon solubility, by using common laboratory reagents like water (cold,hot), dil. HCl, dil. NaOH, dil. $NaHCO_3$, 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 should 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, Benzoic acid/Anthracene; Glucose/Biphenyl; Benzoic acid/Benzophenone; Urea/Benzophenone. **Use of pH paper** is recommended.

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.

CEMA-CC-1-2-TH : (Credits: Theory-04, Practicals-02)

PHYSICAL CHEMISTRY-1 **Theory(40 Lectures)**

Kinetic Theory and Gaseous state

(20 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)

Transport processes

(08 Lectures)

Diffusion : 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 (with derivation); principle of determination of viscosity coefficient of liquids by falling sphere method and using Ostwald's viscometer. Temperature variation of viscosity of liquids and comparison with that of gases. Relation between viscosity coefficient of a gas and mean free path.

Chemical kinetics

(12 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; Rate-determining step and steady-state approximation – explanation with suitable examples; Opposing reactions, consecutive reactions and parallel reactions (with explanation of kinetic and thermodynamic control of products; all steps first order)

Role of Temperature : Temperature dependence of rate constant; Arrhenius equation, energy of activation;

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

Reference Books

1. Levine, I. N. *Physical Chemistry*, 6th Edition McGraw-Hill India
2. Castellan, G. W. *Physical Chemistry*, Narosa
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Kapoor K.L, A Text Book Of Physical Chemistry , McGraw Hill India

5. Engel, T. & Reid, P. *Physical Chemistry*, 3rd Edition Pearson India
6. Atkins, P. W. & Paula, J. de *Atkins' Physical Chemistry*, 10th Edition Oxford University Press
7. Maron, S. & Prutton *Physical Chemistry*
8. Ball, D. W. *Physical Chemistry*, Thomson Press
9. Mortimer, R. G. *Physical Chemistry*, Elsevier
10. Laidler, K. J. *Chemical Kinetics*, Pearson
11. Glasstone, S. & Lewis, G.N. *Elements of Physical Chemistry*
12. Rakshit, P.C., *Physical Chemistry* Sarat Book House
13. Moore, W. J. *Physical Chemistry*, Orient Longman

ORGANIC CHEMISTRY-IB

Theory (20 Lectures)

Stereochemistry I

(17 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, molecular chirality and centre of chirality; asymmetric and dissymmetric molecules; enantiomers and diastereomers; 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.

General Treatment of Reaction Mechanism II (03 Lectures)

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

Reference Books

1. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

3. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
4. Carey, F. A., Giuliano, R. M. *Organic Chemistry*, Eighth edition, McGraw Hill Education, 2012.
5. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London, 1994.
6. Nasipuri, D. *Stereochemistry of Organic Compounds*, Wiley Eastern Limited.
7. Clayden, J., Greeves, N. & Warren, S. *Organic Chemistry*, Second edition, Oxford University Press, 2012.
8. Keeler, J., Wothers, P. *Chemical Structure and Reactivity – An Integrated approach*, Oxford University Press.
9. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
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.

CEMA-CC-1-2-P: **(45 Lectures)**

**** During examination marks of the experiments will be set in 2:1 ratio for Physical and Organic experiments respectively.**

1) PHYSICAL CHEMISTRY: P (1) LAB

(30 Lectures)

Experiment 1: Study of kinetics of decomposition of H_2O_2

Experiment 2: Study of kinetics of acid-catalyzed hydrolysis of methyl acetate

Experiment 3: Study of viscosity of unknown liquid (glycerol, sugar) with respect to water.

Experiment 4: Study of the variation of viscosity with the concentration of the solution

Experiment 5: 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*. 9th Ed., Freeman (2016)
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

2) ORGANIC CHEMISTRY: O (1B) LAB

(15 Lectures)

Determination of boiling point of common organic liquid compounds [ANY FIVE]*n*-butyl alcohol, cyclohexanol, ethyl methyl ketone, cyclohexanone, acetylacetone, isobutyl methyl ketone, isobutyl alcohol, acetonitrile, benzaldehyde and acetophenone. [Boiling points of the chosen organic compounds should preferably be within 180°C].

SEMESTER-2

CEMA-CC-2-3-TH :

(Credits: Theory-04, Practicals-02)

ORGANIC CHEMISTRY-2

Theory: 60 Lectures

StereochemistryII (20 Lectures)

Chirality arising out of stereoaxis: stereoisomerism of substituted cumulenes with even and odd number of double bonds; chiral axis in allenes, spiro compounds, alkylidenecycloalkanes and biphenyls; related configurational descriptors (R_a/S_a); atropisomerism; racemisation of chiral biphenyls.

Concept of prostereoisomerism: prostereogenic centre; concept of (*pro*)ⁿ-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.

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 III

(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; comparison between nucleophilicity and basicity; 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; 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 β -secondary kinetic isotopic effect (k_H/k_D); principle of microscopic reversibility; Hammond's postulate.

Substitution and Elimination Reactions (20 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[systems: alkyl halides, allyl halides, benzyl halides, alcohols, ethers, epoxides, α -halocarbonyls]; 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 (with hetero atoms and aryl groups); role of crown ethers and phase transfer catalysts.

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.

Reference Books

1. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
 2. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
 3. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
 4. Carey, F. A., Giuliano, R. M. *Organic Chemistry*, Eighth edition, McGraw Hill Education, 2012.
 5. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London, 1994.
 6. Nasipuri, D. *Stereochemistry of Organic Compounds*, Wiley Eastern Limited.
 7. Clayden, J., Greeves, N. & Warren, S. *Organic Chemistry*, Second edition, Oxford University Press, 2012.
 8. Keeler, J., Wothers, P. *Chemical Structure and Reactivity – An Integrated approach*, Oxford University Press.
 9. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
 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.
 13. Maskill, H., *Mechanisms of Organic Reactions*, Oxford Chemistry Primer, Oxford University Press.
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CEMA-CC-2-3-P: **(45Lectures)**

Organic Preparations

A. The following reactions (**any eight**) 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. Brine mediated benzoylation of amines/amino acids.
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.

CEMA-CC-2-4-TH :

(Credits: Theory-04, Practicals-02)

INORGANIC CHEMISTRY-2

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 (σ and π bond approach).

Chemical Bonding-II

(30 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_2 , Li_2 , Be_2 , B_2 , C_2 , N_2 , O_2 , F_2 , and their ions wherever possible; Heteronuclear molecular orbitals: CO, NO, NO^+ , CN^- , HF, BeH_2 , CO_2 and H_2O . 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.

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.

Reference Books

1. Lee, J. D. *Concise Inorganic Chemistry*, 5th Ed., Wiley India Pvt. Ltd., 2008.
2. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity* 4th 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* 3rd 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, 5th 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.

CEMA-CC-2-4-P:(45 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

SEMESTER-3

CEMA-CC-3-5-TH :

(Credits: Theory-04, Practicals-02)

PHYSICAL CHEMISTRY-2

Theory: 60 Lectures

Chemical Thermodynamics I

(10 Lectures)

1st 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 , ΔU and ΔH 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 ; Adiabatic flame temperature.

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; 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; Physical concept of Entropy; Entropy is a measure of the microscopic disorder of the system. 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

Systems of Variable Composition:

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs-Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases. Activities and activity coefficients. Fugacity and fugacity coefficient.

Applications of Thermodynamics – I

(06 Lectures)

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; 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- (eg. dimerization of benzene in benzoic acid). Solvent Extraction.

ELECTROCHEMISTRY:

(24 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. 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) Ionic equilibrium:

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). Determination of hydrolysis constant conductometrically. Buffer solutions; derivation of Henderson equation and its applications; buffer capacity, buffer range, buffer action . 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

(iii) Electromotive Force: 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, Thermodynamic derivation of 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 and glass electrodes

Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers; Potentiometric titrations (acid-base, redox, precipitation)

Reference Books

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

CEMA-CC-3-5-P:(45 Lectures)

Experiment 1: Conductometric titration of an acid (strong, weak/ monobasic, dibasic, and acid mixture) against strong base.

Experiment 2: Study of saponification reaction conductometrically

Experiment 3: Verification of Ostwald's dilution law and determination of K_a of weak acid

Experiment 4: Potentiometric titration of Mohr's salt solution against standard $K_2Cr_2O_7$ and $KMnO_4$ solution

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

Experiment 6: Determination of heat of neutralization of a strong acid by a strong base

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*. 9th Ed., Freeman (2016)

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

CEMA-CC-3-6-TH :

(Credits: Theory-04, Practicals-02)

INORGANIC CHEMISTRY-3

Theory: 60 Lectures

Chemical periodicity

(15 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.

Chemistry of s and p Block Elements

(30 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.

Noble Gases:

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

Inorganic Polymers:

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

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.

Reference Books

1. Lee, J. D. *Concise Inorganic Chemistry*, 5th Ed., Wiley India Pvt. Ltd., 2008.
2. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity* 4th 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* 3rd 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, 5th 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.

CEMA-CC-3-6-P:(45 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.
5. Al(III) in Fe(III) and Al(III) in a mixture

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)

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)₃ (aluminiumoxinate).
4. Estimation of chloride.

Reference Books

3. Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis* 6th Ed., Pearson, 2009.
4. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015

CEMA-CC-3-7-TH :

(Credits: Theory-04, Practicals-02)

ORGANIC CHEMISTRY-3

Theory: 60 Lectures

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, halogenation, hydrohalogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, epoxidation, *syn* and *anti*-hydroxylation, ozonolysis, addition of singlet and triplet carbenes; Simmons-Smith cyclopropanation reaction; 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.

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-carbonelectrophiles (reactions: chloromethylation,

Gatterman-Koch, Gatterman, Houben-Hoesch, Vilsmeier-Haack, Reimer-Tiemann, Kolbe-Schmitt); *Ips*o substitution.

Nucleophilic aromatic substitution: addition-elimination mechanism and evidences in favour of it; S_N1 mechanism; cine substitution (benzyne mechanism), structure of benzyne.

Carbonyl and Related Compounds (30 Lectures)

Addition to C=O: structure, reactivity and preparation of carbonyl compounds; mechanism (with evidence), reactivity, equilibrium and kinetic control; formation of hydrates, cyanohydrins 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, LiAlH₄, NaBH₄, 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 α-H of C=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, SeO₂ (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 and silyl enol ethers) in connection with alkylation, acylation and aldol type reaction.

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

Substitution at sp² carbon (C=O system): mechanism (with evidence): B_{AC}2, A_{AC}2, A_{AC}1, A_{AL}1 (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 -COX; directed ortho metalation of arenes using organolithiums, conjugate addition by Gilman cuprates; Corey-House synthesis; abnormal behaviour of Grignard reagents; comparison of reactivity among Grignard, organolithiums and organocopper reagents; Reformatsky reaction; Blaise reaction; concept of *umpolung*.

Reference Books

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

2. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
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.
7. Clayden, J., Greeves, N. & Warren, S. *Organic Chemistry*, Second edition, Oxford University Press, 2012.
8. Graham Solomons, T.W., Fryhle, C. B. *Organic Chemistry*, John Wiley & Sons, Inc.
9. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
10. March, J. *Advanced Organic Chemistry*, Fourth edition, Wiley.
11. Jenkins, P. R., *Organometallic Reagents in Synthesis*, Oxford Chemistry Primer, Oxford University Press.
12. Ward, R. S., *Bifunctional Compounds*, Oxford Chemistry Primer, Oxford University Press.

CEMA-CC-3-7-P:(45 Lectures)

A. 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

B. 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. 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.
6. Arthur, I. Vogel, *Quantitative Organic Analysis*, Pearson
7. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015

SEMESTER-4

CEMA-CC-4-8-TH :

(Credits: Theory-04, Practicals-02)

ORGANIC CHEMISTRY-4

Theory: 60 Lectures

Nitrogen compounds(12 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, 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(14 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 Hauser rearrangement, Fischer-Hepp rearrangement, N-azo to C-azo rearrangement, Bamberger rearrangement, Orton rearrangement and benzidine rearrangement.

The Logic of Organic Synthesis(14 Lectures)

Retrosynthetic analysis: disconnections; synthons, donor and acceptor synthons; natural reactivity and *umpolung*; latent polarity in bifunctional compounds: 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); diastereoselectivity: addition of nucleophiles to C=O adjacent to a stereogenic centre: Felkin-Anh model.

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, α,β -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 $\equiv$ C, C $\equiv$ 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; choice of solvent and internal standard; 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; 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. Warren, S. *Organic Synthesis the Disconnection Approach*, John Wiley and Sons.
13. Warren, S., *Designing Organic Synthesis*, Wiley India, 2009.
14. Carruthers, W. *Modern methods of Organic Synthesis*, Cambridge University Press.
15. Willis, C. A., Wills, M., *Organic Synthesis*, Oxford Chemistry Primer, Oxford University Press

CEMA-CC-4-8-P:(45 Lectures)

Experiment: Qualitative Analysis of Single Solid Organic Compounds

1. Detection of special elements (N, S, Cl, Br) by Lassaigne's test
2. Solubility and classification (solvents: H₂O, 5% HCl, 5% NaOH and 5% NaHCO₃)
3. Detection of the following functional groups by systematic chemical tests: aromatic amino (-NH₂), aromatic nitro (-NO₂), amido (-CONH₂, including imide), phenolic -OH, carboxylic acid (-COOH), carbonyl (distinguish between -CHO and >C=O); only one test for each functional group is to be reported.
4. Melting point of the given compound
5. Preparation, purification and melting point determination of a crystalline derivative of the given compound.
6. 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

1. Vogel, A. I. *Elementary Practical Organic Chemistry*, Part 2: *Qualitative Organic Analysis*, 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. Clarke, H. T., *A Handbook of Organic Analysis (Qualitative and Quantitative)*, Fourth Edition, CBS Publishers and Distributors (2007).
5. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015.

CEMA-CC-4-9-TH :

(Credits: Theory-04, Practicals-02)

PHYSICAL CHEMISTRY 3

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, CO₂, 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

Foundation of Quantum Mechanics

(25 Lectures)

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

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 Vector representation of wave function. Orthonormality of wave function.

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; Complete set of Eigenfunctions. Expansion of Eigenfunctions.

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.

Crystal Structure

(15 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

Reference Books

1. Levine, I. N. *Physical Chemistry*, 6th Edition, McGraw-Hill India
2. Castellan, G. W. *Physical Chemistry*, Narosa
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Kapoor K.L, *A Text Book Of Physical Chemistry*, McGraw Hill India
5. Engel, T. & Reid, P. *Physical Chemistry*, 3rd Edition, Pearson India
6. Atkins, P. W. & Paula, J. de *Atkins' Physical Chemistry*, 10th Edition, Oxford University Press
7. Maron, S. & Prutton, *Physical Chemistry*
8. Ball, D. W. *Physical Chemistry*, Thomson Press
9. Mortimer, R. G. *Physical Chemistry*, 2nd Edition, Elsevier
10. Atkins, P. W. *Molecular Quantum Mechanics*, 5th edition, Oxford
11. Levine, I. N. *Quantum Chemistry*, 7th Edition, Pearson India
12. Sannigrahi A.B, *Quantum Chemistry*, 2nd Edition, Books and Allied Pvt Ltd.
13. Denbigh, K. *The Principles of Chemical Equilibrium* Cambridge University Press
14. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill

CEMA-CC-4-9-P : (45 Lectures)

Experiment 1: Kinetic study of inversion of cane sugar using a Polarimeter (Preferably Digital)

Experiment 2: Study of Phase diagram of Phenol-Water system.

Experiment 3: Determination of partition coefficient for the distribution of I_2 between water and CCl_4

Experiment 4: Determination of pH of unknown solution (buffer), by colour matching method

Experiment 5: pH-metric titration of acid (mono- and di-basic) against strong base

Experiment 6 : pH-metric titration of a tribasic acid against strong base.

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*. 9th Ed., Freeman (2016)
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

CEMA-CC-4-10-TH

(Credits: Theory-04, Practicals-02)

INORGANIC CHEMISTRY-4

Theory: 60 Lectures

Coordination Chemistry-II

(30 Lectures)

VB description and its limitations. Elementary Crystal Field Theory: splitting of d^n 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^n 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 $3d^1$ to $3d^9$ ions. Racah parameter. Selection rules for electronic spectral transitions; spectrochemical series of ligands; charge transfer spectra (elementary idea).

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.

Reference Books

1. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity 4th 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 6th Ed.* 1999., Wiley.
4. Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry 4th 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).

CEMA-CC-4-10-P (45 Lectures)

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)

Instrumental Techniques

1. Measurement of 10Dq by spectrophotometric method.
2. Determination of λ_{max} of $[\text{Mn}(\text{acac})_3]$ and $[\text{Fe}(\text{acac})_3]$ complexes.

Reference Books

1. Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis* 6th Ed., Pearson, 2009.
2. *Inorganic Synthesis*, Vol. 1-10.

SEMESTER-5

CEMA-CC-5-11-TH :

(Credits: Theory-04, Practicals-02)

PHYSICAL CHEMISTRY - 4

Theory: 60 Lectures

Quantum Chemistry II

(30 Lectures)

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 .

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 (ϕ part only), 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 wavefunctions, 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,

3rd 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. Levine, I. N. *Physical Chemistry*, 6th Edition McGraw-Hill India
2. Castellan, G. W. *Physical Chemistry*, Narosa
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Kapoor K.L, A Text Book Of *Physical Chemistry*, McGraw Hill India
5. Engel, T. & Reid, P. *Physical Chemistry*, 3rd Edition Pearson India
6. Atkins, P. W. & Paula, J. de *Atkins' Physical Chemistry*, 10th Edition Oxford University Press
7. Levine, I. N. *Quantum Chemistry*, 7th Edition, Pearson India
8. Maron, S. & Prutton *Physical Chemistry*
9. Ball, D. W. *Physical Chemistry*, Thomson Press
10. Mortimer, R. G. *Physical Chemistry*, Elsevier
11. Glasstone, S. & Lewis, G.N. *Elements of Physical Chemistry*
12. Rakshit, P.C., *Physical Chemistry* Sarat Book House
14. Klotz, I.M., Rosenberg, R. M. *Chemical Thermodynamics: Basic Concepts and Methods*, Wiley
15. Sannigrahi A.B, *Quantum Chemistry*, 2nd Edition, Books and Allied Pvt Ltd.
16. Atkins, P. W. *Molecular Quantum Mechanics*, 5th edition, Oxford
17. Moore, W. J. *Physical Chemistry*, Orient Longman
18. Nash, L. K. *Elements of Statistical Thermodynamics*, Dover
19. V. Rajaraman, *Computer Oriented Numerical Methods*, PHI Learning, 2013
20. V. Rajaraman, *Computer Programming in FORTRAN 77*, Prentice Hall, 1997
21. Martin Cwiakala, *Schaum's Outline of Programming with FORTRAN 77*, 1995

CEMA-CC-5-11-P : (45 Lectures)

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

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

CEMA-CC-5-12-TH :

(Credits: Theory-04, Practicals-02)

ORGANIC CHEMISTRY - 5

Theory: 60 Lectures

Carbocycles and Heterocycles

(16 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 and phenanthrene and their derivatives.

Heterocyclic compounds: Biological importance of heterocycles referred in the syllabus; 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, quinoline: Skraup, isoquinoline: Bischler-Napieralski synthesis.

Cyclic Stereochemistry

(10 Lectures)

Alicyclic compounds: concept of I-strain (Baeyer's strain theory); 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.

Pericyclic reactions

(08 Lectures)

Mechanism, stereochemistry, regioselectivity in case of

Electrocyclic reactions: FMO approach involving 4π - and 6π -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.

Carbohydrates

(14 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 $-\text{CH}_2\text{OH}$ 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.

Biomolecules

(12 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 and '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.

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

CEMA-CC-5-12-P:(45 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 mixture of dyes
4. Paper chromatographic separation of a mixture containing 2/3 amino acids
5. Paper chromatographic separation of a mixture containing 2/3 sugars

B. Spectroscopic Analysis of Organic Compounds

1. Assignment of labelled peaks in the ^1H NMR spectra of the known organic compounds explaining the relative δ -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, $\text{C}\equiv\text{C}$, $\text{C}\equiv\text{N}$ 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-Dimethylbenzonitrile (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.

SEMESTER- 6

CEMA-CC-6-13-TH:

(Credits: Theory-04, Practicals-02)

INORGANIC CHEMISTRY-5

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 Na^+ , K^+ , Mg^{2+} , Ca^{2+} , $\text{Fe}^{3+/2+}$, $\text{Cu}^{2+}/^+$, and Zn^{2+}). Metal ion transport across biological membrane Na^+/K^+ -ion pump. Dioxygen molecule in life. Dioxygen management proteins: Haemoglobin, Myoglobin, Hemocyanine and Hemerythrin. Hydrolytic enzymes: carbonate bicarbonate buffering system and carbonic anhydrase and carboxyanhydrase A. 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. π -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 4th 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 6th 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.

CEMA-CC-6-13-P: (45 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: Na^+ , K^+ , Ca^{2+} , Sr^{2+} , Ba^{2+} , Al^{3+} , Cr^{3+} , $\text{Mn}^{2+}/\text{Mn}^{4+}$, Fe^{3+} , $\text{Co}^{2+}/\text{Co}^{3+}$, Ni^{2+} , Cu^{2+} , Zn^{2+} , Pb^{2+} , Cd^{2+} (Demo), Bi^{3+} (Demo), $\text{Sn}^{2+}/\text{Sn}^{4+}$, $\text{As}^{3+}/\text{As}^{5+}$, $\text{Sb}^{3+}/\text{Sb}^{5+}$ (Demo), NH_4^+ , Mg^{2+} (Demo).

Anion Radicals: F^- , Cl^- , Br^- , BrO_3^- , I^- , IO_3^- , SCN^- , S^{2-} , SO_4^{2-} , NO_3^- , NO_2^- , PO_4^{3-} , AsO_4^{3-} , 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: $\text{Al}_2\text{O}_3(\text{ig})$, $\text{Fe}_2\text{O}_3(\text{ig})$, $\text{Cr}_2\text{O}_3(\text{ig})$, SnO_2 , SrSO_4 , BaSO_4 , CaF_2 , 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

CEMA-CC-6-14-TH:

(Credits: Theory-04, Practicals-02)

PHYSICAL CHEMISTRY-5

Theory: 60 Lectures

Molecular Spectroscopy

(25 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, Diatomic vibrating rotator, P, Q, R branches

Electronic Spectroscopy: Potential energy curves (diatomic molecules), Frank-Condon principle and vibrational structure of electronic spectra; Frank Condon factor. 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: Classical Treatment. Rotational Raman effect; Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion

Photochemistry and Theory of reaction rate:

(15 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_2 - Br_2 reaction, dimerisation of anthracene; photosensitised reactions, quenching; Role of photochemical reactions in biochemical processes, chemiluminescence

Collision theory of reaction rate (detailed treatment). Lindemann theory of unimolecular reaction; Outline of Transition State theory (classical treatment) . Primary Kinetic Salt Effect.

Surface phenomenon

(15 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);

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); Stability of colloids and zeta potential; Micelle formation

Dipole moment and polarizability:

(05 Lectures)

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. Levine, I. N. *Physical Chemistry*, 6th Edition , McGraw-Hill India
2. Castellan, G. W. *Physical Chemistry*, Narosa
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Kapoor K.L, A Text Book Of *Physical Chemistry* , McGraw Hill India
5. Engel, T. & Reid, P. *Physical Chemistry*, 3rd Edition ,Pearson India
6. Atkins, P. W. & Paula, J. de *Atkins' Physical Chemistry*, 10th Edition, Oxford University Press
7. Maron, S. & Prutton , *Physical Chemistry*
8. Ball, D. W. *Physical Chemistry*, Thomson Press
9. Mortimer, R. G. *Physical Chemistry*, 2nd Edition, Elsevier
10. Banwell, C. N. *Fundamentals of Molecular Spectroscopy*, Tata-McGraw-Hill
11. Barrow, G. M. *Molecular Spectroscopy*, McGraw-Hill
12. Hollas, J.M. *Modern Spectroscopy*, Wiley India
13. McHale, J. L. *Molecular Spectroscopy*, Pearson Education
14. Wayne, C. E. & Wayne, R. P. *Photochemistry*, OUP
15. Brown, J. M. *Molecular Spectroscopy*, OUP

CEMA-CC-6-14-P: (45 Lectures)

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

Experiment 2: Determination of the indicator constant of an acid base indicator spectrophotometrically

Experiment 3: Verification of Beer and Lambert's Law for 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: Determination of CMC of a micelle from Surface Tension Measurement.

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.

DISCIPLINE SPECIFIC ELECTIVE COURSES

Semester 5

1. Any one from DSEA-1 and DSEA-2
2. Any one from DSEB-1 and DSEB-2

Semester 6

3. Any one from DSEA-3 and DSEA-4
4. Any one from DSEB-3 and DSEB-4

DSE-A

DSE A-1: MOLECULAR MODELLING AND 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- DSE A-1: MOLECULAR MODELLING & DRUG DESIGN (45 Lectures)

- i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.
- ii. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.
- iii. Visualize the electron density and electrostatic potential maps for LiH, HF, N₂, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
- iv. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- v. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- vi. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
- vii. (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- viii. Arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
- ix. (a) Compare the optimized bond angles H₂O, H₂S, H₂Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.

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

Reference Books:

- 1) A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
- 2) J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.

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

DSE-A-2: APPLICATIONS OF COMPUTERS IN CHEMISTRY

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Computer Programming Basics (FORTRAN): (Lectures: 20)

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: (Lectures: 15)

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-A-2: APPLICATIONS OF COMPUTERS IN CHEMISTRY

(45 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_{sp} and K_{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 a 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

DSE-A-3: GREEN CHEMISTRY AND CHEMISTRY OF NATURAL PRODUCTS

(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: (16 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.
- Green solvents–supercritical fluids, water as a solvent for organic reactions, ionic liquids, PEG, solventless processes.
- Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy.
- Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry.

Examples of Green Synthesis/ Reactions and some real world cases: (20lectures)

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. Green counterpart of common organic reactions: Aldol, Friedel-Crafts, Michael, Knoevenagel, Cannizzaro, benzoin condensation and Dieckmann condensation.
5. Rearrangement reactions by green approach: Fries rearrangement, Claisen rearrangement, Beckmann rearrangement, Baeyer-Villiger oxidation.

Future Trends in Green Chemistry:

(12 Lectures)

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

Alkaloids**(5 Lectures)**

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

Terpenes**(3 Lectures)**

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

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. & Tinneland, M. *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).
5. Lancaster, M. *Green Chemistry: An Introductory Text* RSC Publishing, 2nd Edition, 2010.
6. Ahluwalia, V. K & Kidwai, M. R. *New Trends in Green Chemistry*, Anamalaya Publishers, 2005.
7. Finar, I. L. *Organic Chemistry (Volume 2)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

PRACTICALS-DSE-A-3: GREEN CHEMISTRY**(45 Lectures)**

(Any **SIX** of the following list)

1. Acetylation of primary amine (preparation of acetanilide).
2. [4+2] Cycloaddition reaction (Diels-Alder reaction between furan and maleic anhydride).
3. Preparation of biodiesel from vegetable/waste cooking oil.
4. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
5. Pinacol-pinacolone rearrangement reaction (preparation of benzopinacolone).
6. Solid state synthesis of benzoic acid from benzil.
7. Benzoin condensation using thiamine hydrochloride as a catalyst instead of potassium cyanide.
8. Green multicomponent synthesis (three component coupling).
9. Base catalysed aldol condensation (synthesis of dibenzal propanone from benzaldehyde and acetone).
10. Bromination of *trans*-stilbene using bromide/bromate mixture.
11. Preparation and characterization of gold nanoparticles using tea leaves.
12. Extraction of D-limonene from orange peel using liquid carbon dioxide.

13. Electrophilic aromatic substitution reaction (nitration of salicylic acid).
14. Green radical coupling reaction.

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 C ISBN 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, 2nd 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-A4: ANALYTICAL METHODS IN CHEMISTRY **(Credits: Theory-04, Practicals-02)**

Theory: 60 Lectures

Optical methods of analysis:

(30 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: (7 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 pK_a 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* 6thEd., Pearson, 2009.
2. Willard, H.H. *et al.*: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.

3. Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
4. Harris, D.C.: *Exploring Chemical Analysis*, 9th 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.

PRACTICALS-DSE-A-4: ANALYTICAL METHODS IN CHEMISTRY (45 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* 6th Ed., Pearson, 2009.
2. Willard, H.H. *et al.*: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
4. Harris, D.C. *Exploring Chemical Analysis*, 9th 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.

DSE-B

DSE-B-1: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE

(Credits: Theory-04, Practicals-02)

Theory: 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. Hightechnology 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 (Arand 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).

PRACTICALS-DSE B-1: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE**(45 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. Sharma, B.K. & Gaur, H. *Industrial Chemistry*, Goel Publishing House, Meerut (1996).

DSE B-2: NOVEL INORGANIC SOLIDS

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Synthesis and modification of inorganic solids: (10 Lectures)

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

Inorganic solids of technological importance: (10 Lectures)

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

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

Nanomaterials:

(10 Lectures)

Overview of nanostructures and nanomaterials: classification.

Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control

of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires. Bio-inorganic nanomaterials, DNA and nanomaterials, natural and artificial nanomaterials, bionano composites.

Introduction to engineering materials for mechanical construction: (10 Lectures)

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

Composite materials(10 Lectures)

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

Speciality polymers:

(10 Lectures)

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

Reference Books:

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

PRACTICAL – DSEB-2: NOVEL INORGANIC SOLIDS

(45 Lectures)

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

Reference Book

- Fahan, *Materials Chemistry*, Springer (2004).
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DSE-B-3: POLYMER CHEMISTRY

(Credits: Theory-04, 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: (08 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*, 4th Ed. Wiley, 2004.
3. F.W. Billmeyer: *Textbook of Polymer Science*, 2nd 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.

PRACTICALS – DSE- B-3: POLYMER CHEMISTRY

(45 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_2 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*, 3rd Ed., Oxford University Press, 1999.
 2. H.R. Allcock, F.W. Lampe & J.E. Mark, *Contemporary Polymer Chemistry*, 3rd ed. Prentice-Hall (2003)
 3. F.W. Billmeyer, *Textbook of Polymer Science*, 3rd ed. Wiley-Interscience (1984)
 4. J.R. Fried, *Polymer Science and Technology*, 2nd ed. Prentice-Hall (2003)
 5. P. Munk & T.M. Aminabhavi, *Introduction to Macromolecular Science*, 2nd ed. John Wiley & Sons (2002)
 6. L. H. Sperling, *Introduction to Physical Polymer Science*, 4th ed. John Wiley & Sons (2005)
 7. M.P. Stevens, *Polymer Chemistry: An Introduction* 3rd ed. Oxford University Press (2005).
 8. Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).
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DSE B-4 : Dissertation

(Credits: 06)

In a total of 105 lecture hours, a student has to carry out research /review on a topic as assigned by the respective college. A project report and digital presentation will be required for the assessment of the student at the end of the semester.

SKILL ENHANCEMENT COURSES

SEC-A [SEMESTER 3]

SEC 1 – 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. (08 Lectures)

2.Differential

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

(04 Lectures)

3. **Probability:** Permutations, combinations and theory of probability (03 Lectures)

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.

(04 Lectures)

5. Qualitative and quantitative aspects of analysis:

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals. (03 Lectures)

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. **(08 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 2 – ANALYTICAL CLINICAL BIOCHEMISTRY

(Credits: 2 Lectures:30)

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

Isolation and characterization of polysaccharides.

Proteins: Classification, biological importance; Primary and secondary and tertiary structures of proteins: α -helix and β -pleated sheets, Isolation, characterization, denaturation of proteins.

Enzymes: Nomenclature, Characteristics (mention of Ribozymes), 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.

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-B [SEMESTER 4]

SEC 3 – 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), antiloprosy (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.

SEC-4 PESTICIDE CHEMISTRY

(Credits: 02, 30 Lectures)

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

Hands on Practicals

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

Reference Book:

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

GENERAL ELECTIVE COURSE IN CHEMISTRY

Course Structure (B.Sc. General)

Course Credits

Theory+ Practical

Core Course (CC)

Theory (12 Papers of 4 credits each)	$12 \times 4 = 48$
Practical (12 Papers of 2 credits each)	$12 \times 2 = 24$

Discipline Specific Elective Course* (DSE)

Theory (6 Papers of 4 credits each)	$6 \times 4 = 24$
Practical (6 Papers of 2 credits each)	$6 \times 2 = 12$

Ability Enhancement Compulsory Course (AECC)

(2 Papers of 2 credits)	$2 \times 2 = 4$
Environmental Science	
English/MIL Communication	

Skill Enhancement Elective Course (SEC)

(4 Papers of 2 credits)	$4 \times 2 = 8$
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Total credit	120
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B.SC. (GENERAL) CHEMISTRY [CEM-G]

CORE /GENERIC COURSES

SEM	COURSE CODE [CEM-G]	PAPER
1	CC1/GE1	PAPER 1
2	CC2/GE2	PAPER 2
3	CC3/GE3	PAPER 3
4	CC4/GE4	PAPER 4

DISCIPLINE SPECIFIC ELECTIVE [DSE] COURSES

DSE- A

DSEA-1 : Novel Inorganic Solids

DSEA-2: Inorganic Materials of Industrial Importance

DSE-B

DSEB-1 : Green Chemistry and Chemistry of Natural Products

DSEB-2: Analytical Methods in Chemistry

SKILL ENHANCEMENT COURSES [SEC]

SEC(A): (Any one either in semester III or V)

SEC1 : Basic Analytical Chemistry

SEC2– Analytical Clinical Biochemistry

SEC(B) (Any one either in semester IV or VI)

SEC 3 – PHARMACEUTICALS CHEMISTRY

SEC 4 - PESTICIDE CHEMISTRY

CC1/ GE 1:

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Kinetic Theory of Gases and Real gases

Concept of pressure and temperature; Collision of gas molecules; Collision number and mean free path. 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 Deviation of real gases from ideal behavior; compressibility factor; Boyle temperature; Andrew's and Amagat's plots; van der Waals equation and its features; Existence of critical state, Critical constants in terms of van der Waals constants; Law of corresponding states.

Liquids

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)

Chemical Kinetics

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-life and differential method. Temperature dependence of rate constant; Arrhenius equation, energy of activation;

Atomic Structure

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

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

Brönsted–Lowry concept, conjugate acids and bases, relative strengths of acids and bases, effects of substituent and solvent, differentiating and leveling 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.

Fundamentals of Organic Chemistry

Electronic displacements: inductive effect, resonance and hyperconjugation; nucleophiles and electrophiles; reactive intermediates: carbocations, carbanions and free radicals.

Stereochemistry

Different types of isomerism; geometrical and optical isomerism; concept of chirality and optical activity (upto two carbon atoms); asymmetric carbon atom; 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* (only one chiral carbon atoms) and *E/Z* nomenclature.

Nucleophilic Substitution and Elimination Reactions

Nucleophilic substitutions: S_N1 and S_N2 reactions; eliminations: E1 and E2 reactions (elementary mechanistic aspects); Saytzeff and Hofmann eliminations.

CC1/GE 1 Practical: 45 Lectures

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with KMnO₄.
3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO₄.
4. Estimation of Fe (II) ions by titrating it with K₂Cr₂O₇ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using Na₂S₂O₃.
6. Estimation of Fe(II) and Fe(III) in a given mixture using K₂Cr₂O₇ solution.

CC2/GE 2:

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Chemical 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 , ΔU and ΔH 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, Kirchhoff's equations. Statement of the second law of thermodynamics; Concept of heat reservoirs and heat engines; Carnot cycle; Physical concept of Entropy; 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:

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

Solutions

Ideal solutions and Raoult's law, deviations from Raoult's law – non-ideal solutions; Vapour pressure-composition and temperature-composition curves of ideal and non-ideal solutions; Distillation of solutions; Lever rule; Azeotropes
Nernst distribution law and its applications, solvent extraction

Phase Equilibria

Phases, components and degrees of freedom of a system, criteria of phase equilibrium; Gibbs Phase Rule; Derivation of Clausius – Clapeyron equation and its importance in phase equilibria; Phase diagrams of one-component systems (water and CO_2)

Solids

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;

Aliphatic Hydrocarbons

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.

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:* addition of bromine, addition of HX [Markownikoff's (with mechanism) and anti-Markownikoff's addition], hydration, ozonolysis.

Alkynes: (up to 5 Carbons). *Preparation:* acetylene from CaC_2 ; by dehalogenation of tetra halides and dehydrohalogenation of vicinal dihalides.

Reactions: formation of metal acetylides, hydration reaction.

Error Analysis and Computer Applications

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.

Redox reactions

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

CC2/GE 2 Practical: 45 Lectures

Experiment 1: Study of kinetics of acid-catalyzed hydrolysis of methyl acetate

Experiment 2: Study of kinetics of decomposition of H_2O_2 (Clock Reaction)

Experiment 3: Study of viscosity of unknown liquid (glycerol, sugar) with respect to water.

Experiment 4: Determination of solubility of sparingly soluble salt in water, in electrolyte with common ions and in neutral electrolyte (using common indicator)

Experiment 5: Preparation of buffer solutions and find the pH of an unknown buffer solution by colour matching method

Experiment 6: Determination of surface tension of a liquid using Stalagmometer

CC3/GE 3:

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

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Chemical Bonding and Molecular Structure

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

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

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

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

Comparative study of p-block elements:

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

Transition Elements (3d series)

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

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

Coordination Chemistry

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

ELECTROCHEMISTRY

1) Ionic Equilibria

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

2) Conductance

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 Moving-boundary method

3) Electromotive force

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;

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)

Aromatic Hydrocarbons

Benzene: Preparation: from phenol, by decarboxylation, from acetylene. *Reactions:* electrophilic substitution reaction (general mechanism); nitration (with mechanism), halogenations (chlorination and bromination), and Friedel-Crafts reaction (alkylation and acylation) (up to 4 carbons on benzene).

Organometallic Compounds

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

Aryl Halides

Preparation: (chloro- and bromobenzene): from phenol, Sandmeyer reaction and effect of nitro substituent (activated nucleophilic substitution)

CC3/GE 3 Practical: 45 Lectures

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

Cation Radicals: Na^+ , K^+ , Ca^{2+} , Sr^{2+} , Ba^{2+} , Al^{3+} , Cr^{3+} , $\text{Mn}^{2+}/\text{Mn}^{4+}$, Fe^{3+} , $\text{Co}^{2+}/\text{Co}^{3+}$, Ni^{2+} , Cu^{2+} , Zn^{2+} , Pb^{2+} , $\text{Sn}^{2+}/\text{Sn}^{4+}$, NH_4^+ .

Anion Radicals: F^- , Cl^- , Br^- , BrO_3^- , I^- , IO_3^- , SCN^- , S^{2-} , SO_4^{2-} , NO_3^- , NO_2^- , PO_4^{3-} , AsO_4^{3-} , BO_3^{3-} , $\text{CrO}_4^{2-} / \text{Cr}_2\text{O}_7^{2-}$

CC4/GE 4:

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Alcohols, Phenols and Ethers

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, oxidation (alkaline KMnO_4 , acidic dichromate).

Diols: 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, Schotten –Baumann reaction, Fries rearrangement and Claisen rearrangement.

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

Carbonyl Compounds

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, NaHSO_3 , $\text{NH}_2\text{-G}$ 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

Carboxylic Acids and Their Derivatives

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.

Carboxylic acid derivatives (aliphatic): (up to 5 carbons). *Preparation*: acid chlorides, anhydrides, esters and amides from acids; *Reactions*: Interconversion among acid derivatives. *Reactions*: Claisen condensation; Perkin reaction.

Amines and Diazonium Salts

Amines (aliphatic and aromatic): strength of organic bases; *Preparation*: from alkyl halides, Hofmann degradation;

Reactions: with HNO_2 (distinction of 1°, 2°- and 3°- 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

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

Carbohydrates: classification and general properties; glucose and fructose: constitution; osazone formation; oxidation-reduction reactions; ascending (Kiliani –Fischer method) and descending (Ruff's method) in monosaccharides (aldoses only); mutarotation

Crystal Field Theory

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

Jahn-Teller distortion, Square planar coordination

Quantum Chemistry & Spectroscopy

Spectroscopy and its importance in chemistry. Wave-particle duality. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter. Types of spectroscopy. Difference between atomic and molecular spectra

Postulates of quantum mechanics, quantum mechanical operators.

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

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

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

Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels. Selection rules, IR spectra of diatomic molecules.

CC4/GE 4 Practical: 45 Lectures

1. 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: H₂O, dil. HCl, dil. NaOH)

Experiment C: Detection of functional groups: Aromatic-NO₂, Aromatic -NH₂, -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.

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. 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. N. G. Mukherjee *Quantum Chemistry, molecular Spectroscopy and Photochemistry*. Archana Publishing Center, (2010).
6. Bahl, B.S., Bahl, A., Tuli, G.D., *Essentials of Physical Chemistry* S. Chand & Co. Ltd.
7. Palit, S. R., *Elementary Physical Chemistry* Book Syndicate Pvt. Ltd.
8. N. G. Mukherjee, *Elementary Physical Chemistry* Archana Publishing Center, (2014).
9. Mandal, A. K. *Degree Physical and General Chemistry* Sarat Book House
10. Pahari, S., *Physical Chemistry* New Central Book Agency
11. Palit, S.R., *Practical Physical Chemistry* Science Book Agency
12. Mukherjee, N.G., *Selected Experiments in Physical Chemistry* J. N. Ghose & Sons
13. Dutta, S.K., *Physical Chemistry Experiments* Bharati Book Stall
14. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015
15. Banerjee, S. P. *A Text Book of Analytical Chemistry*, The New Book Stall.
16. Gangopadhyay, P. K. *Application Oriented Chemistry*, Book Syndicate.
17. Mondal, A. K & Mondal, S. *Degree Applied Chemistry*, Sreedhar Publications
18. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
19. Ghosal, Mahapatra & Nad, *An Advanced Course in Practical Chemistry*, New Central
20. Sethi, A. *Conceptual Organic Chemistry*; New Age International Publisher.
21. Parmar, V. S. *A Text Book of Organic Chemistry*, S. Chand & Sons.
22. Madan, R. L. *Organic Chemistry*, S. Chand & Sons.
23. Wade, L. G., Singh, M. S., *Organic Chemistry*, Pearson.

24. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
25. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
26. Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.
27. Cotton, F.A. & Wilkinson, G. *Basic Inorganic Chemistry*, Wiley.
28. Shriver, D.F. & Atkins, P.W. *Inorganic Chemistry*, Oxford University Press.
29. Wulfsberg, G. *Inorganic Chemistry*, Viva Books Pvt. Ltd.
30. Rodgers, G.E. *Inorganic & Solid State Chemistry*, Cengage Learning India Ltd., 2008.

DSE (A)

Any one from the following

DSE A-1: NOVEL INORGANIC SOLIDS

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Synthesis and modification of inorganic solids: (10 Lectures)

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

Inorganic solids of technological importance: (10 Lectures)

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

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

Nanomaterials: (10 Lectures)

Overview of nanostructures and nanomaterials: classification.

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

Introduction to engineering materials for mechanical construction: (10 Lectures)

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

Composite materials (10 Lectures)

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

Speciality polymers: (10 Lectures)

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

materials, manufacturing and applications.

Reference Books:

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

PRACTICAL – DSEA-1 : NOVEL INORGANIC SOLIDS

(45 Lectures)

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

Reference Book

- Fahan, *Materials Chemistry*, Springer (2004).
-

DSE-A-2: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE

(Credits: Theory-04, Practicals-02)

Theory: 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. Hightechnology 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 (Arand 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).

PRACTICALS-DSE A2 LAB INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE

(45 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).

DSE(B)

Any one from the following

DSE-B1: GREEN CHEMISTRY AND CHEMISTRY OF NATURAL PRODUCTS

(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: (16 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.
- Green solvents–supercritical fluids, water as a solvent for organic reactions, ionic liquids, PEG, solventless processes.
- Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy.
- Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry.

Examples of Green Synthesis/ Reactions and some real world cases: (20lectures)

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. Green counterpart of common organic reactions: Aldol, Friedel-Crafts, Michael, Knoevenagel, Cannizzaro, benzoin condensation and Dieckmann condensation.
5. Rearrangement reactions by green approach: Fries rearrangement, Claisen rearrangement, Beckmann rearrangement, Baeyer-Villiger oxidation.

Future Trends in Green Chemistry: (12 Lectures)

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

Alkaloids

(5 Lectures)

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

Terpenes

(3 Lectures)

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

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. & Tinneland, M. *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).
5. Lancaster, M. *Green Chemistry: An Introductory Text* RSC Publishing, 2nd Edition, 2010.
6. Ahluwalia, V. K & Kidwai, M. R. *New Trends in Green Chemistry*, Anamalaya Publishers, 2005.

PRACTICALS-DSE-B1 LAB GREEN CHEMISTRY

(45 Lectures)

1. Acetylation of primary amine (preparation of acetanilide).
2. [4+2] Cycloaddition reaction (Diels-Alder reaction between furan and maleic anhydride).
3. Preparation of biodiesel from vegetable/waste cooking oil.
4. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
5. Pinacol-pinacolone rearrangement reaction (preparation of benzopinacolone).
6. Solid state synthesis of benzilic acid from benzil.
7. Benzoin condensation using thiamine hydrochloride as a catalyst instead of potassium cyanide.
8. Green multicomponent synthesis (three component coupling).
9. Base catalysed aldol condensation (synthesis of dibenzal propanone from benzaldehyde and acetone).
10. Bromination of *trans*-stilbene using bromide/bromate mixture.
11. Preparation and characterization of gold nanoparticles using tea leaves.
12. Extraction of D-limonene from orange peel using liquid carbon dioxide.
13. Electrophilic aromatic substitution reaction (nitration of salicylic acid).
14. Green radical coupling reaction.

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, WashingtonDC (2002).
 3. Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, WashingtonDC (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 CISBN978-93-81141-55-7 (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, 2nd 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.
 9. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
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DSE-B2: ANALYTICAL METHODS IN CHEMISTRY

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Optical methods of analysis:

(30 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:

(7 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 pK_a 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* 6th Ed., Pearson, 2009.
2. Willard, H.H. *et al.: Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
4. Harris, D.C.: *Exploring Chemical Analysis*, 9th 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.

PRACTICALS- DSE-B-2: ANALYTICAL METHODS IN CHEMISTRY (45 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* 6th Ed., Pearson, 2009.
- 2. Willard, H.H. et al.: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- 3. Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
- 4. Harris, D.C. *Exploring Chemical Analysis*, 9th 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.

SKILL ENHANCEMENT COURSES (SEC)

SEC(A)

SEC1 : Basic Analytical Chemistry

(Credits2 , 30 lectures)

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

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

- a. Determination of pH of soil samples.
- b. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

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

- a. Determination of pH, acidity and alkalinity of a water sample.
- b. Determination of dissolved oxygen (DO) of a water sample.

Analysis of food products: Nutritional value of foods, idea about food processing and food preservations and adulteration.

- a. Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
- b. Analysis of preservatives and colouring matter.

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

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

Ion-exchange: Column, ion-exchange chromatography etc.

Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Analysis of cosmetics: Major and minor constituents and their function

- a. Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.
- b. Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

Suggested Applications (Any one):

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

Suggested Instrumental demonstrations:

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

Reference Books:

1. Willard, H. H. *Instrumental Methods of Analysis*, CBS Publishers.
2. Skoog & Lerry. *Instrumental Methods of Analysis*, Saunders College Publications, New

York.

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

SEC2 – ANALYTICAL CLINICAL BIOCHEMISTRY

(Credits: 2 Lectures:30)

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

Isolation and characterization of polysachharides.

Proteins: Classification, biological importance; Primary and secondary and tertiary structures of proteins: α -helix and β -pleated sheets, Isolation, characterization, denaturation of proteins.

Enzymes: Nomenclature, Characteristics (mention of Ribozymes), 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.

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.

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(B)

SEC 3 – 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), antiloprosy (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.

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.

SEC 4 - PESTICIDE CHEMISTRY

(Credits: 02)

30 Lectures

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

Reference Book:

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