NEP Syllabus (Semester I – IV)
SoC, UoH

Semester (I)

1. Structural Chemistry and Thermodynamics I (3 credits)

(i) Structural Chemistry (1.5 credits)

Atomic Structure: Quantum mechanical concepts – Quantum numbers - Orbital shapes and sizes [4 h] Periodic properties - Slater's rules [3 h] Chemical Bonding: VB and MO approaches for homonuclear and heteronuclear diatomic molecules - Concept of HOMO and LUMO - VSEPR theory - Shapes of molecules [5 h] Ionic Solids: Close packing- Radius ratio rule and crystal coordination number - Examples of MX and MX_2 types of ionic solids - Lattice energy (e.g., NaCl) [4 h] Metallic Bonding: Theories of bonding in metals - Free electron, VB and Band theories [2 h] Weak Interactions: Hydrogen bonding and van der Waals interactions [2 h]

Suggested Readings:

1. F. A. Cotton, G. Wilkinson and P. L. Gaus, Basic Inorganic Chemistry, Third Edition, Wiley India Edition, 2007 (Reprinted), ISBN: 9789354246913
2. J. D. Lee, Concise Inorganic Chemistry, 5th Edition [Paperback, OUP, 2008), ISBN-10: 8126515546

(ii) Thermodynamics (1.5 credits)

Equations of state, ideal and real gas laws, critical phenomena (3h); Fundamental Concepts of Thermodynamics: definitions of variables (intensive/extensive), functions (state/path) and systems (1h); Heat, Work, Internal Energy, Enthalpy and the First Law of Thermodynamics, Thermochemistry, Joule-Thomson effect (8h); Entropy and the Second and Third Laws of Thermodynamics, heat engines, Carnot cycle, reversible and irreversible changes, Clausius inequality, Maxwell relations (6h); (total: 18h)

Suggested Readings:

1. Physical Chemistry (6th edition) by Ira N. Levine
2. Physical Chemistry (3rd edition) by Thomas Engel & Philip Reid
3. Physical Chemistry (9th edition) by Peter Atkins and Julio de Paula
4. Physical Chemistry (3rd edition) by Gilbert Castellan

Semester (II)

1. Basics of Analytical and Organic Chemistry [3 credits]

(i) Organic Chemistry (1.5 credits)

Bonding and physical properties of organic molecules [8h]
Nomenclature of simple organic compounds. Hybridization, Inductive, hyper-conjugation, bond-polarization, resonance, mesomeric effects, tautomerism and weak intermolecular interactions. Aromaticity, anti-aromaticity and homo-aromaticity. Physical properties of bond distance, bond angles, dipole moment, melting point and

boiling point in terms of structure and bonding. Acids and bases: Effect of structure, substituent and solvent on acidity and basicity.

Basic reaction mechanism and intermediates [4h]
Homolytic & heterolytic bond cleavages and formations, representation of mechanistic steps using arrow formalism. Reactive intermediates: carbocation (carbenium and carbonium ions), carbanions, radicals, carbenes: generation, structure, stability and selected examples on their reactivity (elementary aspects).
Stereochemistry [6h]
Representation of molecules in saw-horse, Fischer, flying-wedge and Newman formulae and their inter translations, and molecular chirality. Configurational isomerism: Stereogenicity, D/L and R/S notations, *threo*, *erythro* & *meso* and *syn*/*anti* nomenclature. Optical activity of chiral compounds: specific rotation, optical purity (enantiomeric excess), racemic compounds - resolution. Conformation – ethane, cyclohexane.

Suggested Readings:

1. P. Y. Bruice, Organic Chemistry, 8th Edition, Pearson Education (2016).
2. T. W. Graham Solomons and C. B. Fryhle, Organic Chemistry, 10th edition, Wiley.
3. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Education (2010).
4. I. L. Finar, Organic Chemistry, Vol-1, 6th edition, Pearson Education.
5. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, Wiley.

(ii) Analytical Chemistry (1.5 credits)

1. Errors in Chemical Analysis – [4 h]

Errors and types - Accuracy and precision -, Absolute and relative errors, Determinate (systematic) and indeterminate (random) errors - Statistical treatment of random errors – source and distribution - Sample and populations - Mean, deviations and standard deviation - Propagation of errors - Criteria for rejection of a data (q-test) - Significant figures and computation rules for significant figures - Method of least squares

2. Basics of titrimetry – [2 h]

Terminology – Concentration (molarity, normality weight percentage concepts) -Equivalence point and end point -Primary and secondary standards - Equilibrium constant and meaning of quantitative reactions - Conditions for reactions used in titrations - Some examples of stoichiometric calculations

3. Acid-base Titrations – [2 h]

Acid-base indicators -Theory of acid base indicators - Calculation of pH values at different stages of the acid-base titration and titration curve

4. Complexometric Titrations – [2 h]

Complexometric titrations – Principles - Effects of complexing agents and their advantages Examples including EDTA based titration and titration curve -Definition of pM^+ ($-\log M^+$), Back and blank titration with examples - Direct and indirect determinations -Masking and demasking with examples

5. Precipitation Titrations – [2 h]

Precipitation titrations - Mohr, Volhard and Fajans methods with examples and indicator theory.

6. Gravimetric Method of Analysis – [2 h]

Principle and use with example - von Weimarn's theory of relative supersaturation –Digestion - Ostwald ripening – Coprecipitation, Postprecipitation, Precipitation from homogeneous solution -Organic precipitants

7. Redox titrations [3 h]

Reduction potentials and electrochemical series - Redox indicators and their use in volumetric analysis - Back titrations and indirect titrations - Iodometry and iodimetry, Examples of titration from other redox systems.

8. Electrochemical methods of analysis [3 h]

Electrodes and electrochemical cell -Standard electrodes - Glass electrode and pH measurement – Electrogravimetry- Potentiometric titrations

Suggested Readings:

(1) "Qualitative Analysis" – R. A. Day and A. L. Underwood, 6th edition, Pearson Education India (2015).
(2) "Fundamentals of Analytical Chemistry" – Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch, 9th Edition, Cengage Learning (2013)

2. Qualitative & Quantitative Inorganic Analysis Lab (1.5 credits)

1. Observation of reactions of common cations and anions.

2. Semimicro analysis of salts and Group separation of cations: Following radicals (anions and cations) analysis will be conducted in this course.

   Anions or Acid radicals: Nitrate (NO_3^-), Sulfate (SO_2^-), Nitrite (NO_2^-), Chloride (Cl^-), Bromide (Br^-), Iodide (I^-) Acetate (CH_3COO^-), Carbonate (CO_3^{2-}), Sulphide (S^{2-}), Bromate (BrO_3^-), Iodate (IO_3^-), Phosphate (PO_4^{3-}).

   Cation or Basic Radicals: Silver (Ag^+), Lead (Pb^{2+}), Copper (Cu^{2+}), Cadmium (Cd^{2+}), Tin (Sn^{2+}), Iron (Fe^{3+}), Chromium (Cr^{3+}), Cobalt (Co^{2+}), Nickel (Ni^{2+}), Manganese (Mn^{2+}), Zinc (Zn^{2+}), Barium (Ba^{2+}), Strontium (Sr^{2+}), Calcium (Ca^{2+}), Sodium (Na^+), Potassium (K^+), Ammonium (NH_4^+).

3. Use of Volumetric Apparatus: Burette, Pipette, Measuring jar and Standard flask - Determination of accuracy and precision of volumetric measurements.

4. Titrimetry: Acid-base, Redox and Complexometric titrations - The following experiments will be conducted:
   (a) Acid-base titration: Primary and secondary standards - Standardization of sodium hydroxide with potassium hydrogen phthalate
   (b) Acid-base titration: Standardization of hydrochloric acid - Estimation of sodium carbonate - Estimation of sodium carbonate and sodium bicarbonate in a mixture.
   (c) Redox titration: Standardization of potassium permanganate - Estimation of iron.
   (d) Redox titration: Indirect titration - iodometry – Standardization of sodium thiosulphate - estimation of copper.
   (e) Redox titration: Back titration - Standardization of ammonium ferrous sulphate using potassium dichromate and estimation of barium as chromate by back titration with potassium dichromate.

5. Gravimetry: Determination of water of hydration and estimation of chloride and barium.

Suggested Readings:

1. Lab manual provided by teacher
2. Vogel's Qualitative Inorganic Analysis, 7th Edition
3. Vogel's Textbook of Quantitative Inorganic Analysis, 4th Edition, Revised by J. Bassett, R. C. Denney, G. H. Jeffery, and J. Mendham, Longmann (1982);
4. Quantitative Analysis, R. A. Day and A. L. Underwood, 6th Edition, Pearson Education India (2015).

Semester (III)

1. Basic Inorganic Chemistry and Thermodynamics II [3 credits]

(i) Inorganic Chemistry (1.5 credits)

1. Nuclear Chemistry: Nuclear binding energy –Radioactivity -Artificial isotopes -Nuclear fission -Synthesis of trans-uranium elements -Separation of radioactive isotopes -Nuclear fusion -Application of isotopes -Radiocarbon dating [4 h]

2. Acids & Bases: Various definitions of acids and bases - Factors affecting strength of acids and bases - K_a, K_b, K_w and pH - Henderson's equation -Hydrolysis of salts - Common ion effect - Brønsted and Lewis acids and bases - Gas phase versus solution phase acidity, HSAB principle - Surface acidity [6 h]

3. Non-aqueous Solvents: Properties of a solvent for functioning as an effective reaction medium - Types of solvents and general characteristics of liquid NH_3, SO_2, HF, H_2SO_4, BF_3 and N_2O_4 - An introduction to superacids - Ionic liquids and supercritical fluids [5 h]

4. Chemistry of selected s- & p-block elements: Hydrogen bonds - Hydrates and water clathrates - Alkali metal solution in liquid ammonia - Complexation of alkali metals by crown ethers and cryptands - Alkali metal anions -Diborane – Structure and bonding - Noble gas compounds. [5 h]

Suggested Readings:

1. Catherine E. Housecroft and Alan G. Sharpe, Inorganic Chemistry, Second Edition, Pearson Education Limited, 2005.
2. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 3rd Edition, Pearson Education, 2004.

(ii) Thermodynamics II (1.5 credits)

Prerequisite: Basics of Thermodynamics

Gibbs and Helmholtz energy, chemical potential, free energy and entropy of mixing of ideal gas, ideal solutions, mixture of ideal solutions, colligative properties: boiling point, freezing point, solubility and osmosis (5h)

Chemical equilibrium: Equilibrium constant of reaction of ideal gas and its temperature dependence: van't Hoff equation, Le Chatelier principle, Fugacity and the Equilibrium Constant of real gas (3h).

Phase equilibrium: Phase transitions of pure substances: phase stability, boundary and phase rule, examples of phase diagrams; thermodynamics of phase transition: Clausius-Clapeyron equation, order of phase transition; phase diagrams of binary systems, lever rule, liquid-liquid and solid-liquid phase diagrams (6h).

Non-ideal solutions: Activity and activity coefficient, activity coefficient in concentration scales, activity of electrolyte, ionic activity and coefficient. (4h) (total: 18h)

Suggested Readings:

1. Physical Chemistry (6th edition) by Ira N. Levine
2. Physical Chemistry (3rd edition) by Gilbert Castellan
3. Physical Chemistry (3rd edition) by Thomas Engel & Philip Reid
4. Physical Chemistry (9th edition) by Peter Atkins and Julio de Paula

(2) Preparation and Analysis of Organic Compounds Lab (1.5 Credits)

Prerequisite: None

Purification of organic compounds by crystallization and determination of melting point
Characterisation of organic functional groups.
Preparation of organic compounds using classical organic reactions like nitration, bromination, acetylation, condensation and oxidation/reduction.
Estimation of selected organic compounds.

Suggested Readings:

1. Donald L. Pavia, Gary M. Lampman, George S. Kriz and Randall G. Engel, A Microscale Approach to Organic Laboratory Techniques, 6th Edition, Cengage Learning, ELBS (2016).
2. A.I. Vogel, Textbook of Practical Organic Chemistry, 4th edition.
3. Laboratory manual.

Semester (IV)

1. Chemistry of Organic Functional Groups (3 credits)

Prerequisite: Basic organic chemistry or equivalent

Chemistry of alkanes and arenes, alkenes, alkynes, halides, alcohols, phenols, ethers, carbonyls, carboxylic acids and their derivatives and amines – Synthesis and reactivity.

Detailed syllabus

Alkanes: Preparation - Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. *Reactions:* Free radical Substitution: Halogenation. [1]

Alkenes: Preparation - Elimination reactions, dehydration and dehydrohalogenation of alkyl halides (Saytzeff's rule); *cis*-alkenes (Partial catalytic hydrogenation) and *trans*-alkenes (Birch reduction). Reactions: *cis*-addition (alk. $KMnO_4$) and *trans*-addition (bromine), Addition of HX (Markownikoff's and *anti*-Markownikoff's addition), hydration, ozonolysis, oxymecuration-demercuration and hydroboration. [3]

Alkynes: Preparation - acetylene from CaC_2 and conversion into higher alkynes, by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides. Reactions: formation of metal acetylides, addition of bromine and alkaline $KMnO_4$. [1]

Aromatic hydrocarbons: Preparation - from phenol, by decarboxylation and from acetylene. Reactions - electrophilic substitution: nitration, halogenation and sulfonation. Friedel-Craft's reaction - alkylation and acylation. Side chain oxidation of alkyl benzenes. [4]

Alkyl Halides: Types of nucleophilic substitution (S_N1, S_N2 and S_Ni) reactions.
Preparation: from alkenes and alcohols. Reactions: solvolysis, halide displacement reactions. Williamson's ether synthesis and elimination *vs* substitution. [4]

Aryl Halides: Preparation: from phenol, Sandmeyer & Gattermann reactions. Reactions: aromatic nucleophilic substitutions. Benzyne formation and reactions. [2]

Alcohols: Preparation - Preparation of 1°, 2° & 3° alcohols and 1,2-diols: using Grignard reagent, ester hydrolysis, reduction of aldehydes, ketones, carboxylic acid and esters. Reactions: With alkali metals, HX (Lucas test), esterification, oxidation (with PCC, alk. $KMnO_4$, acidic dichromate, conc. HNO_3). Oppeneauer oxidation Diols: oxidation of diols. Pinacol-Pinacolone rearrangement.
Phenols: Preparation - Cumene hydroperoxide method, from diazonium salts. Reactions - Electrophilic substitution and named reactions.
Ethers (aliphatic and aromatic): Cleavage of ethers. [4]

Carbonyls: Preparation - from other functional groups. Reactions – with HCN, ROH, $NaHSO_3$, amine derivatives. Cannizzaro's reaction, Benzoin condensation. Named reactions involving carbonyls.
Chemistry of □-carbon of carbonyls - pKa of □□C-H, keto-enol tautomerism. Halogenation, haloform reaction, aldol reaction. Reformatsky reaction, Michael reaction, Robinson annulation, Knoevenagel condensation, Claisen ester condensation, Perkin reaction, Stobbe condensation, Darzens reaction, acyloin condensation, McMurry coupling Wittig reaction and other named reactions.
Malonic and acetoacetic esters: Characteristic reactions of active methylene group, synthetic uses of malonic, acetoacetic and cyanoacetic ester. [10]
Carboxylic acids: Preparation by acid and base mediated hydrolysis of esters.

Reactions: Hell–Vohlard-Zelinsky reaction and reactions involving carboxylic functionality.
Carboxylic acid derivatives: acid chlorides, anhydrides, esters and amides from acids and their interconversion. Reactions - condensation reactions. [3]

Amines: Preparation - from alkyl halides, Gabriel's Phthalimide synthesis, Hofmann bromamide reaction and by reduction reactions. Reactions - Hofmann degradation, qualitative tests for amines, Schotten – Baumann Reaction. Electrophilic substitution: nitration, bromination, sulfonation.
Diazonium compounds – preparation and reactions. [4]

Suggested Readings:

1. P. Y. Bruice, Organic Chemistry, 8th Edition, Pearson Education (2016).
2. T. W. Graham Solomons and C. B. Fryhle, Organic Chemistry, 10th edition, Wiley.
3. F. A. Carey and R. M. Giuliano, Organic Chemistry, 10th Edition, McGraw Hill Education (2017).
4. J. McMurry, *Organic Chemistry,* 9th Edition, Cengage Learning (2016).
5. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Education (2010).

2. Kinetics, Transport Phenomenon & Surface Chemistry (3 credits)

Prerequisite: Basics of thermodynamics, differential equations

Transport phenomenon:

Motion of molecules in gas: kinetic theory of gas, collision of gas molecules, mean free path, collision on wall, Maxwell speed distribution, effusion, diffusion equation and coefficient (4h)

Motion of molecules in liquids: conductivity of electrolytic solution, ionic mobility, migration of ions, strong and weak electrolytes, conductometric titrations, transport number and measurement, Grotthuss mechanism (4h); ion activities and Debye-Hückel theory (qualitative descriptions only): Debye-Hückel limiting law, Debye-Hückel theory for concentrated solution (3h); theory of electrolytic conductance (qualitative description only): ionic atmosphere, electrophoretic effect, Wien effect and Debye-Falkenhagen effect (2 h).

Electrochemical Cells: Daniell Reversible and irreversible cells, cell representations and half-cell reactions, Thermodynamics of electrochemical systems: Nernst equations, varieties of electrodes, standard electrode potential. (3 h)

Type of boundary between half cells and Liquid junction potentials, Concentration cells, Applications of EMF measurements-potentiometric titrations, determination of activity coefficient, composition of complex ions, solubility product, measurement of pH and pKa (Hydrogen, Quinhydrone, Glass electrodes), Polarization, Overvoltage. (4 h)

Chemical Kinetics: Extent of reaction, order of a chemical reaction, rate equations, differential and integrated rate laws: first, second and n^{th} order reactions; unimolecular reactions, chain and photochemical reactions (5 h); Approximate methods: quasi steady state approximation and quasi-equilibrium approximation; consecutive and simultaneous reactions; temperature dependence of rate constant; Arrhenius equation, energy of activation; basic ideas of collision theory and transition state theory(4 h); Homogeneous catalysis: acid-base catalysis; enzyme catalysis; Michaelis-Menten equation, Lineweaver-Burk plot (2 h)

Heterogeneous catalysis: Adsorption and desorption of molecules, physisorption and chemisorption, Langmuir Isotherm, BET and other isotherms, dissociative adsorption, temperature dependence of adsorption, sticking probability; unimolecular and bimolecular reaction: Langmuir-Hinshelwood and Eley-Rideal mechanisms (6 h)

Surfaces and interfaces: surface tension – Young's equation and contact angles – surface Gibbs function and Gibbs equation – surfactants and surface pressure – surface double layer and potential (3 h)

Suggested Readings:

1. Physical Chemistry (9th edition) by Peter Atkins and Julio de Paula
2. Physical Chemistry (3rd edition) by Thomas Engel & Philip Reid
3. Physical Chemistry (6th edition) by Ira N. Levine
4. Physical Chemistry (3rd edition) by Gilbert Castellan
5. An Introduction to Electrochemistry by Samuel Glasstone

3. Physical Chemistry Lab (1.5 credits)

List of experiments:

1. Molecular weight of a polymer (viscometry)
2. Stoichiometry of a complex (Job's method)
3. Conductometric titrations (acid-base and precipitation reaction)
4. Thermodynamics: Heat of solution (calorimetry)
5. Phase diagram of a 2-component system
6. pKa of amino acid (pH titration)
7. Solubility product
8. Partition coefficient
9. Kinetics: Rate constant of acid catalyzed ester hydrolysis

Suggested Readings: Lab manual (http://chemistry.uohyd.ac.in/Files/Other/CY202-Manual.pdf)