Semester-VI

Chemistry MAJOR
Course code: CHEM6011 (3 and 4 Years)
Course title: Inorganic Chemistry (Theory)

Credit: 4

Course objective:
Development of knowledge for several basic and advanced topics of inorganic chemistry

Course outcome:
The course will help the students to develop a complete knowledge on metallurgy, lanthanides & actinides, bio-inorganic chemistry, organometallic chemistry as well as reaction kinetics & mechanism

1. **General Principles of Metallurgy**

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

   10 hours

2. **Lanthanoids and Actinoids**

   General comparison on electronic configuration, oxidation states, colour, spectral and magnetic properties; lanthanide contraction, separation of lanthanides (ion-exchange method only). *8 hours*

3. **Bioinorganic Chemistry**

   Elements of life: essential and beneficial elements, major, trace and ultratrace elements. Role of metal ions (specially Na^+, K^+, Mg^{2+}, Ca^{2+}, $Fe^{3+/2+}$, $Cu^{2+/+}$, and Zn^{2+}) in biological systems. Metal ion transport across biological membrane Na^+/K^+-ion pump, Oxygen transport in biological systems: haemoglobin, myoglobin, hemocyanine and hemerythrin. Electron transfer proteins: Cytochromes and ferredoxins, hydrolytic enzymes: carbonate bicarbonate buffering system, carbonic anhydrase and carboxyanhydrase A, biological nitrogen fixation, photosynthesis: photosystem-I and photosystem-II, toxic metal ions and their effects, chelation therapy (examples only), Pt and Au complexes as drugs (examples only), metal dependent diseases (examples only).

10 hours

4. **Organometallic Chemistry**

(i) 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 properties 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.

(ii) *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.

20 hours

5. Reaction Kinetics and Mechanism

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 reactions, ligand field effects and reaction rates, mechanism of substitution in octahedral complexes. *12 hours*

Reference Books

1. Arnikar, H. J. Essentials of Nuclear Chemistry, New Age International, 1995.
2. Lee, J. D. Concise Inorganic Chemistry 5th Ed., John Wiley and sons 2008.

3. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006.
4. Douglas, B.E. and McDaniel, D.H. Concepts & Models of Inorganic Chemistry Oxford, 1970.
5. Cotton, F.A., Wilkinson, G., & Gaus, P.L. Basic Inorganic Chemistry 3rd Ed.; Wiley India.
6. Miessler, G. L., Fischer, P. J., Tarr, D. A., Inorganic Chemistry, Pearson, 5th Edition.
7. Banerjee, S. P., Comprehensive Coordination Chemistry, Books & Allied Pvt. Ltd., 2019
8. Mingos, D.M.P., Essential trends in inorganic chemistry. Oxford University Press (1998).
9. Atkins, P., Overton, T., Rourke, J., Weller, M., Armstrong, F,. Shriver & Atkins, Inorganic Chemistry, Fifth Edition, Oxford University Press.

Chemistry MAJOR
Course code: CHEM6012 (3 and 4 Years)
Course title: Organic Chemistry (Theory)

Credit: 4

Course objective:
Development of knowledge for several basic and advanced topics of organic chemistry

Course outcome:
The course will help the students to develop a complete knowledge on organic spectroscopy, cyclic stereochemistry, heterocyclic chemistry as well as introductory concept on green chemistry

1. Organic Spectroscopy

(i) *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 λ_{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 λmax considering conjugative effect, steric effect, solvent effect, effect of pH; effective chromophore concentration: keto-enol systems; benzenoid transitions.

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

(iii) *NMR Spectroscopy*: introduction; nuclear spin; NMR active molecules; basic principles of Proton Magnetic Resonance; equivalent and non-equivalent protons; chemical shift and factors influencing it; ring current effect, anisotropic effects in alkene, alkyne, aldehydes and aromatics;; significance of the terms: up-/downfield, shielded and deshielded protons; spin coupling and coupling constant (1st order spectra); relative intensities offirst-order multiplets: Pascal's triangle; chemical and magnetic equivalence in NMR; elementary idea about non-first-order splitting; 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.

(iv) Applications of IR, UV and NMR spectroscopy for identification of simple organic molecules. *30 hours*

2. Cyclic Stereochemistry

Alicyclic compounds: concept of I-strain; conformational analysis: cyclohexane, mono and disubstituted cyclohexane; symmetry properties and optical activity; 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.

10 hours

3. Heterocyclic chemistry

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 itsvariation; thiophenes: Paal-Knorr synthesis, Hinsberg synthesis; pyridine: Hantzsch synthesis;benzofused 5- and 6-membered rings with one heteroatom: reactivity, orientation and importantreactions (with mechanistic details) of indole, quinoline and isoquinoline; synthesis (includingretrosynthetic approach and mechanistic details): indole: Fischer, Madelung and Reissert;quinoline: Skraup, Doebner- Miller, Friedlander; isoquinoline: Bischler-Napieralski synthesis. *10 hours*

4. Green Chemistry

Twelve principles and goals of green chemistry:

Designing greener processes: Prevention of waste/ by-products; 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.

Green solvents– supercritical carbon dioxide, water as green solvent, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, immobilized solvents.

Examples of Green Synthesis / Reactions and some real-world cases

Green synthesis of adipic acid, Hofmann Elimination, oxidation of toluene and alcohols; Diels-Alder reaction and Decarboxylation reaction, Simmons-Smith reaction, Aldol condensation reaction, Friedel-Crafts, Michael, Knoevenagel, Cannizzaro, Benzoin condensation and Dieckmann condensation.

10 hours

Reference Books

1. Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley, London.
2. Nasipuri, D. Stereochemistry of Organic Compounds, Wiley Eastern Limited.
3. Sengupta, S., Basic Stereochemistry of Organic Molecules, Oxford University Press, 2014.
4. Kalsi, P. S. Stereochemistry Conformation and Mechanism, Eighth edition, New Age International, 2014.
5. Joule, J. A. & Mills, K. Heterocyclic Chemistry, Blackwell Science.
6. Gilchrist, T. L. Heterocyclic Chemistry, 3rd edition, Pearson.
7. Bansal, R. K. Heterocyclic Chemistry, New Age International Publishers.
8. Davies, D. T., Heterocyclic Chemistry, Oxford Chemistry Primer, Oxford University Press.
9. Ahluwalia, V.K., Heterocyclic Chemistry, Narosa Publishing House, 2012.

10. Anastas, P.T. & Warner, J.K., Green Chemistry-Theory and Practical, Oxford University Press (1998).
11. Ryan, M.A. & Tinnesand, M. Introduction to Green Chemistry, American Chemical Society, Washington, 2002.
12. Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2nd Edition, 2010.
13. Ahluwalia, V.K., Green Chemistry: A Textbook, 1st Ed., Narosa Publishing House, 2013
14. Jag Mohan, Organic Spectroscopy: Principles and Applications, 2nd Ed., Narosa Publishing House, 2010.
15. Sharma, YY.R., Elementary Organic Spectroscopy: Principles and Chemical Applications, S. Chand & Company Ltd.
16. Manna, A.K., Organic Molecular Spectroscopy, Books & Allied (P) Ltd.2nd Ed., 2020.
17. Kalsi, P.S., Spectroscopy of Organic Compounds, New Age International Publisher

Chemistry MAJOR
Course code: CHEM6013 (3 and 4 Years)
Course title: Physical Chemistry (Theory)

Credit: 4

Course objective:
Development of knowledge for several basic and advanced topics of physical chemistry

Course outcome:
The course will help the students to develop a complete knowledge on thermodynamic applications, electrical properties of molecules, molecular spectroscopy and photochemistry

1. Applications of Thermodynamics

Condensed phase: Chemical potential of pure solid and pure liquids, ideal solution – definition, Raoult’s law; mixing properties of ideal solutions, chemical potential of a component in an ideal solution; choice of standard states of solids and liquids.

Colligative properties: Vapour pressure of solution; ideal solutions, ideally diluted solutions and colligative properties; Raoult's law; thermodynamic derivation using chemical potential for the four colligative properties, relative lowering of vapour pressure, elevation of boiling point, depression of freezing point and osmotic pressure; applications in calculating molar masses of solutes; abnormal colligative properties for dissociated and associated solutes in solution.

Heterogenous equilibria: Definitions of phase, component and degrees of freedom; phase rule and its derivations; phase diagram for water, CO_2, sulphur

1^{st} order phase transition and Clapeyron equation; Clausius-Clapeyron equation - derivation and use; liquid vapour equilibrium for two component systems.

Binary solutions: ideal solution at fixed temperature and pressure; Nernst distribution law and its applications, principle of fractional distillation; Duhem-Margules equation; Henry's law; Konowaloff's rule; positive and negative deviations from ideal behavior; 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

18 Hours

2. Electrical Properties of Molecules

Ionic equilibria: Chemical potential of an ion in solution; activity and activity coefficients of ions in solution; Debye-Hückel limiting law-brief qualitative description of the postulates involved, qualitative idea of the model, the equation (without derivation) for ion-ion atmosphere interaction potential; calculation of activity coefficient for electrolytes using Debye-Hückel limiting law; derivation of mean ionic activity coefficient from the expression of ion-atmosphere interaction potential; applications of the equation and its limitations.

Electromotive Force: Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry; chemical cells, reversible and irreversible cells with examples; Electromotive force of a cell and its measurement, Nernst equation; standard electrode (reduction) potential and its application to different kinds of half-cells. application of EMF measurements in determining (a) free energy, enthalpy and entropy of a cell reaction, (b) equilibrium constants, and (c) 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; qualitative discussion of potentiometric titrations (acid-base, redox, precipitation).

18 hours

3. Molecular Spectroscopy

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

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

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration.

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

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and lowresolution spectra, different scales, spin-spin coupling and high-resolution spectra

14 hours

4. Photochemistry

Lambert-Beer's law: Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients; Laws of photochemistry, StarkEinstein law of photochemical equivalence quantum yield, actinometry, examples of low and high quantum yields Photochemical Processes: Potential energy curves (diatomic molecules), Frank-Condon principle and vibrational structure of electronic spectra; Bond dissociation and principle of determination of dissociation energy (ground state); Decay of excited states by radiative and non-radiative paths; Pre-dissociation; Fluorescence and phosphorescence, Jablonski diagram

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, photostationary states, chemiluminescence

10 hours

Reference Books

1. Castellan, G. W. Physical Chemistry, Narosa

2. Atkins, P. W. & Paula, J. de Atkins', Physical Chemistry, Oxford University Press.

3. McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press.

4. Levine, I. N. Physical Chemistry, Tata McGraw-Hill.

5. Moore, W. J. Physical Chemistry, Orient Longman.

6. Mortimer, R. G. Physical Chemistry, Elsevier.

7. Engel, T. & Reid, P. Physical Chemistry, Pearson.

8. Maron, S.H., Prutton, C. F., Principles of Physical Chemistry, McMillan.

9. Klotz, I.M., Rosenberg, R. M. Chemical Thermodynamics: Basic Concepts and Method, Wiley.

10. Rastogi, R. P. & Misra, R.R. An Introduction to Chemical Thermodynamics, Vikas Publishing House.

11. Glasstone, S. An Introduction to Electrochemistry, East-West Press.

12. Rakshit, P.C., Physical Chemistry, Sarat Book Distributors, 7th Ed.

13. Kapoor, K.., A Textbook of Physical Chemistry, Volume-4, McGraw Hill Education (India) Pvt. Ltd., 5th Ed.

14. Kapoor, K.., A Textbook of Physical Chemistry, Volume-5, McGraw Hill Education (India) Pvt. Ltd., 5th Ed.

Chemistry MAJOR
Course code: CHEM6014 (3 and 4 Years)
Course title: Inorganic & Physical Chemistry (Practical)

Credit: 4

F.M. 75 (60+ 15)

Course objective:
Development of practical knowledge for several basic and advanced topics of inorganic and physical chemistry
Course outcome:
The course will help the students to develop a complete practical knowledge oninorganic as well as physical chemistry

Inorganic Chemistry experiments (F.M. 30) *60 hours*

I. Volumetric estimation using redox titration:

(a) Estimation of Mohr's salt with standard $KMnO_4$ and $K_2Cr_2O_7$ solution

(b) Estimation of Fe^{+2} and Fe^{+3} (total iron) with standard $KMnO_4$ and $K_2Cr_2O_7$ solution

(c) Estimation of one of the metal ions such as iron, copper, chromium and manganese in a binary

mixture using dichromometry/permanganometry/iodometry as applicable

II. Volumetric estimation using complexometric titration:

Complexometric titration using EDTA for estimation of (a) Ca(II) or Mg(II) in a mixture and (b) total hardness of water sample

III. Colorimetric analysis of (i) Mn(II) in permanganate solution and (ii) Cr(III) in dichromate solution

Physical Chemistry Experiments (F.M. 30) *60 hours*

a. Verification of Beer-Lambert's law for aqueous $KMnO_4$ and $K_2Cr_2O_7$ solutions.

b. Determination of Indicator Constant (K_{In}) of an acid-base indicator colorimetrically.

c. Potentiometric titration of a solution of strong acid with a solution of strong alkali using quinhydrone electrode.

d. Potentiometric titration of a solution of weak acid with a solution of strong alkali and determination of pKa of the weak acid.

e. Potentiometric titration of Mohr's salt solution against standard $K_2Cr_2O_7$ solution

f. Determination of hydrolytic constant (K_h) of ammonium chloride solution pH-metrically.

g. Study the phase diagram of a binary system (phenol-water) and the effect of impurities (e.g., NaCl)

Reference Books

1. Mendham, R.C., Denney, J.D., Baines, M. Thomas and Siva Sankar, B. Vogel's Text Book on Quantitative Chemical Analysis, 6/e, Pearson.

2. Nad, A. K., Mahapatra, B. & Ghosal, A. An Advanced Course in Practical Chemistry, New Central Book Agency, 2007.

3. Das, S.C. Advanced Practical Chemistry, The World Press Pvt. Ltd., 4th Ed. 2010

4. Mukhopadhyay, R. & Chattejee, P. Advanced Practical Chemistry, Books & Allied (P) Ltd., 3rd Ed., 2007.

5. Maity, S. K. & Ghosh, N. K. Physical Chemistry Practical, New Central Book Agency (P) Ltd. 2012