B. SC. IN CHEMISTRY

DETAILED SYLLABUS OF FYUGP SEMESTER-VII

Course Title: Inorganic Chemistry-IV (DSC-16)

Course Code: MAJ-CHM-7.1

Total Credit: 4 (3 Credit Theory + 1 Credit Practical)

Distribution of marks: 70 (End Semester) (45T+25P) + 15 (In-Semester) + 15(HA/S/GD)

Course objective: The aim of this course is to introduce the students with the fundamental concepts of group theory like matrix representation, symmetry elements and operations, reducible and irreducible representation, application of group theory in predicting the IR and Raman active vibrational modes, orbital symmetry and chemical reactions. This course will establish the basic foundation of electronic structure, spectra and magnetic properties of transition and inner-transition metal complexes. Students will also learn the characterization of inorganic compounds by NMR Spectroscopy.

Theory: 3 Credits   Total course hour: 45 hr   Duration of Examination: 2 hr.

Unit-1: Group Theory (10 Lectures)

Symmetry elements and symmetry operations, symmetry groups, molecular dissymmetry and optical activity, symmetry point groups for compounds having co-ordination number 2 to 9, matrix representation of groups, reducible and irreducible representation, the great orthogonality theorem, Direct product representation. Projection operator, symmetry adapted linear combination, vibrational modes as bases for group representation, symmetry selection rules for IR and Raman spectra.

Unit-2: Electronic structure and spectra of transition and inner-transition metal complexes (12 Lectures)

Spectroscopic states, Crystal Field Theory, Russel-Saunders Coupling (L-S Coupling) and Term Symbols, Orgel and Tanabe-Sugano diagrams, selection rules, band intensities and band width, Adjusted Crystal Field Theory, Spectrochemical and Nephelauxetic series, molecular orbital theory of complexes (including complexes with and without π bonding), MO diagrams for octahedral and tetrahedral complexes, Jahn-Teller effect, Charge-transfer spectra (LMCT, MLCT), optical properties of lanthanides and actinides.

Unit-3: Magnetic properties of transition and inner transition metal complexes (15 Lectures)

Types of magnetic behaviour: dia-, para-, ferro- and anti-ferromagnetic compounds, Curie and Curie-Weiss laws, Orbital and spin magnetic moments, spin-orbit coupling, spin only moments of d^n ions and their correlation with effective magnetic moments including orbital contribution; quenching of magnetic moment: super exchange and anti-ferromagnetic interactions, temperature independent paramagnetism, application of Crystal Field Theory to explain magnetic properties, spin-crossover. Thermodynamic effects-hydration, ligation, lattice energy, magnetic properties of lanthanides and actinides.

Unit 4: Physical Characterization of Inorganic Compounds by NMR Spectroscopy (10 Lectures)

Basic principle and spectral display, Application NMR spectroscopy-fundamentals, the contact and pseudo-contact shifts, factors affecting nuclear relaxation, application of H-1, C-13, P-31 and F-19 NMR towards the structural elucidation of metal-organic complexes, an overview of metal nuclides with emphasis on Pt-195 and Sn-119 NMR.).

Practical: 1 Credit **Total course hour: 30 hr** **Duration of Examination: 3 hr**

List of experiments:

1. Gravimetric Analysis:
i. Estimation of nickel (II) using Dimethylglyoxime (DMG).
ii. Estimation of copper as CuSCN
iii. Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$.
iv. Estimation of Al (III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminium oxinate).
2. Estimation of Iron(III) and Copper(II) in a mixture.

Learning outcome:
On completion of this course the students will be able to learn:

(i) The point group a molecule belongs, symmetry species of the normal modes of vibration and their spectroscopic activities. The student will learn how to generate molecular orbitals by symmetry adapted linear combination of atomic orbitals (SALC) which will help one doing quantum chemistry calculation with more ease.

(ii) To interpret electronic spectra of transition metal complexes, understanding the nature of d-d transitions and other charge transfer transitions and their relationship to color.

(iii) The magnetic properties of transition and inner transition metal complexes.

(iv) The physical characterization of some inorganic compounds by NMR Spectroscopy.

(v) The principles of gravimetric analysis, perform accurate quantitative analysis, and apply the method to determine the concentration of analytes in various samples.

(vi) How quantitatively analyze the mixture using techniques like redox titrations and gravimetric methods, understanding the principles of analytical chemistry and achieving accurate results.

Suggested reading:

(1) Bioinorganic photochemistry by G. Stochel. Wiley.
(2) Principles and Applications of Photochemistry by Brian Wardle. Wiley.
(3) Fundamental of Photochemistry by K K Rohatgi-Mukherjee, New Age International Publishers.
(4) Chemical Applications of Group Theory by F. A. Cotton.
(5) Symmetry and Spectroscopy of Molecules by K Veera Reddy.
(6) Asim K. Das Fundamental Concepts of Inorganic Chemistry, Vol. 5, 6, 7.
(7) O. Kahn, Molecular Magnetism.
(8) R. P. Sarkar, General and Inorganic Chemistry (Vol. 2), New Central Book Agency, ed. 3, 2011,
(9) Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006.
(10) Housecroft, C.E. and Sharpe, A.G. (2012) Inorganic Chemistry. 4th Edition, Pearson, Harlow.
(11) Marr, G. and Rockett, R.W. Practical Inorganic Chemistry, Van Nostrand Reinhold. 1972.
(12) Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, 2009.
(13) An Advanced Course in Practical Chemistry by Nad, Mahapatra & Ghosal. Publisher, New Central Book Agency (P) Limited, 2014.

Course Title: Organic Chemistry-IV (DSC-17)

Course Code: MAJ-CHM-7.2

Total Credit: 4 (3 Credit Theory + 1 Credit Practical)

Marks Distribution: 70 (End Semester) (45T+25P) + 15 (In-Semester) + 15 (HA/S/GD)

Course Objective: To introduce advanced concepts in organic chemistry, focusing on key reagents, reaction mechanisms, and their applications in synthesis, medicinal chemistry, and polymer science through integrated theory and practical work.

Prerequisite: A basic foundation in organic chemistry, including knowledge of: Functional groups and their reactivity, Fundamental reaction mechanisms and Basic principles of chemical bonding.

Theory: 3 Credits   Total course hour: 45 hr   Duration of Examination: 2 hr.

Unit 1: Organometallic reagents and Organosulphur compounds (9 Lectures)

Introduction to organometallic Reagents: Fundamental concepts, structure and bonding; Grignard reagents, organolithium compounds, organozinc and organocopper reagents.

Preparation and reactions of thiols, Acidity and nucleophilicity of thiols, Disulfide formation and biological relevance of it, Umpolung of carbonyl compounds using dithiane and synthetic utility
Desulfurization reaction.

Unit 2: Selected Oxidizing and reducing agents used in organic transformations (9 Lectures)

Common oxidizing agents: PCC, PDC (Pyridinium dichromate), $KMnO_4$, OsO_4, m-CPBA, Swern oxidation (DMSO/oxalyl chloride), Dess–Martin periodinane, Ozone (O_3), Woodward and Prevost reactions.

Common reducing agents: $LiAlH_4$, $NaBH_4$, H_2/Pd, Zn/Hg in HCl (Clemmensen reduction), hydrazine/KOH (Wolff–Kishner reduction), Na/NH_3 (Birch reduction), DIBAL-H (Diisobutylaluminium hydride), Lindlar catalyst (Pd/$BaSO_4$ with quinoline), Raney nickel.

Unit 3: C-C and C=C bond formations reactions (9 Lectures)

C–C Bond Forming Reactions: Alkylation of enamines and enolates (kinetic vs thermodynamic); Transition metal-catalyzed C–C bond formation: general mechanisms and key reactions- Heck, Suzuki, Stille, Sonogashira.

C=C Bond Forming Reactions: Pyrolytic syn elimination: thermal elimination mechanisms, ester pyrolysis, xanthate ester pyrolysis (Chugaev reaction), and amine oxide pyrolysis (Cope elimination), stereospecificity and mechanism; Stereoselectivity of Wittig reaction, comparison with Horner-Wadsworth-Emmons reaction; Peterson olefination and Shapiro reaction.

Unit 4: Introduction to Medicinal Chemistry (9 Lectures)

Definition and classification of drugs, prodrugs, History of drug development: Aspirin, paracetamol, sulpha drugs, Receptors, drug-receptor interaction, agonist, antagonist; Chemotherapeutic index & therapeutic index, IC_{50}, EC_{50}, LD_{50} values; Lead compound, structure activity relationship Quantitative structure activity relationships (QSAR).
Drugs of the different pharmacological classes: Antibiotics, Antifungal, Antiviral and anti HIV-AIDS, Antimalarials, Analgesics and antipyretics, Anticancer.

Unit 5: Introduction to Organic Polymers (9 Lectures)

Macromolecules: Characteristics of macromolecules, classification of polymers, polymerisation reaction (addition and condensation), and degree of polymerization. Types of polymers and polymerization process: Addition polymers, stereo controlled dipolymers, condensation polymers, Zeigler-Natta catalyst. Manufacture and application of the following polymers: Natural rubber and synthetic rubber; Synthetic fibres: Polyesters, polyamides; Plastics: Polythenes and polyurethanes; Foaming agents: Plasticisers and stabilizers.

Practical: 1 Credit **Total course hour: 30 hr** **Duration of Examination: 3 hr**

Experiments:

1. Preparation of paracetamol.
2. Separation of a mixture of dyes by Thin Layer Chromatography (TLC).
3. Preparation of Starch-PVA Film
4. Separation and Qualitative Analysis of Two-Component Organic Mixtures
   (a) Preliminary examination: physical properties, ignition test, solubility.
   (b) Detection of extra elements (N, S, halogens) using Lassaigne's test.
   (c) Separation of components based on differential solubility in acid, base, or organic solvents.
   (d) Systematic qualitative analysis of functional groups (carboxylic acids, phenols, amines, alcohols, aldehydes, ketones, esters, etc.).
   (e) Confirmatory tests and derivative preparation.
   (f) Melting/boiling point determination and report writing.

Learning Outcome:

By the end of the course, students will be able to:

- Gain foundational knowledge of organometallic and organosulfur chemistry, including their structures, properties, and synthetic applications.
- Understand the role and mechanism of commonly used oxidizing and reducing agents in organic transformations.
- Acquire conceptual and practical understanding of key carbon-carbon and carbon-carbon double bond forming reactions.
- Develop a basic understanding of medicinal chemistry, including drug classification, design, and drug-receptor interactions.
- Learn the principles of polymer chemistry, types of polymers, polymerization methods, and industrial applications.
- Build practical skills in organic synthesis, compound analysis, and separation techniques through hands-on laboratory work.

Suggested reading:

1. Norman, R.O.C. and Coxon, C. M. Principles of Organic Synthesis, CRC Press, New York, 2009.
2. Carruthers, W. and Coldham, I (2004), Moder Methods of Organic Synthesis, 4th Edition, Cambridge University Press.

3. Clayden, J., Greeves N., Warren, S., Organic Chemistry, Oxford University Press 2nd Ed., 2012.
4. M. B. Smith, J. March, March's Advanced Organic Chemistry: Reactions, Mechanisms,
   and Structure, 2007 John Wiley & Sons, Inc
5. B. Y. Paula, Organic Chemistry, 8th edition, Pearson Education India.
6. F. W. Billmeyer, *Textbook of Polymer Science*, John Wiley & Sons, Inc.
7. V. R.Gowariker, N. V. Viswanathan, &J. Sreedhar, *Polymer Science*, New Age International (P) Ltd. Pub
8. A.I. Vogel: Textbook of Practical Organic Chemistry, 5th edition, Prentice-Hall
9. F. G. Mann & B. C. Saunders, Practical Organic Chemistry, Orient Longman (1960)

Course Title: Physical Chemistry IV (DSC-18)

Course Code: MAJ-CHM-7.3

Total Credit: 4 (3 Credit Theory + 1 Credit Practical)

Distribution of marks: 70 (End Semester) (45T+25P) + 15 (In-Semester) + 15(HA/S/GD)

Course objective: This course aims to deepen the understanding of classical and statistical thermodynamics, focusing on the thermodynamic behavior of mixtures, phase equilibria, and nonideal systems. It integrates statistical mechanics to relate microscopic behavior to macroscopic thermodynamic properties, including entropy, energy distributions, and partition functions. The course also introduces non-equilibrium thermodynamics, emphasizing entropy production, Onsager relations, and real-world applications such as diffusion, electrokinetics, and biological systems.

Theory: 3 Credits   Total course hour: 45 hr   Duration of Examination: 2 hr.

Course Content:

Unit 1: Chemical Thermodynamics (15 Lectures)

Brief review of thermodynamic functions and laws of thermodynamics: Temperature dependence of thermodynamic functions, Experimental determination of thermodynamic functions, Thermodynamic description of mixtures, Gibbs-Duhem equation, Chemical equilibrium, Thermodynamic description of phase transitions, Clapeyron-Claussius equation, Phase diagrams, Thermodynamics of nonideal systems – fugacity and activity concepts, excess properties.

Unit 2: Statistical thermodynamics (15 Lectures)

Concepts of statistical thermodynamics, entropy and probability, ensembles, distribution laws of MB, FD and BE, partition functions and statistical formulation of macroscopic variables.

Use of statistical thermodynamics including calculation of electrical and magnetic properties, and heat capacity of solids, application of BE statistics to helium.

Unit 3: Non-equilibrium thermodynamics (15 Lectures)
Non-equilibrium thermodynamics, thermodynamic criteria for non-equilibrium states, Assumptions of non-equilibrium thermodynamics, uncompensated heat, entropy production and entropy flow, entropy balance, Onsager formalism, relation between forces and fluxes, transformations of generalized fluxes and forces, microscopic reversibility and Onsager's reciprocity relations.
Electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

Practical: 1 Credit **Total course hour: 30 hr** **Duration of Examination: 3 hr**

List of Experiments:

1. Determination of Enthalpy and Entropy of Dissolution (e.g., Benzoic Acid)
2. Phase Diagram Construction for Binary Systems (e.g., Naphthalene–Biphenyl)
3. Diffusion Coefficient Determination (e.g., $KMnO_4$ in Water)

Learning outcome: After completion of the course, the learner shall be able to apply classical thermodynamic principles to mixtures, phase transitions, and chemical equilibria, including nonideal systems. They will interpret and calculate thermodynamic functions, fugacity, activity and excess functions. Students will use statistical thermodynamics to derive macroscopic properties from molecular behaviour, employing MB, FD, and BE statistics. They will analyze non-equilibrium processes, entropy production, and Onsager reciprocity in real systems, including electrokinetic and biological phenomena, enabling advanced analysis and research in physical chemistry.

Suggested reading:

1. Engel, T. and Reid, P. Thermodynamics, Statistical Thermodynamics and Kinetics, 2nd Edn., (Pearson, New Delhi, 2011).
2. Atkins, P. and Paula, J. de. Atkins' Physical Chemistry, 10th Edn., (Oxford University Press, New Delhi, 2014).
3. Kalidas, C. and Sangaranarayanan, M.V. Non-equilibrium Thermodynamics, Principles and applications, (Mcmillan, New Delhi, 2002).
4. Berry, R. Rice S. A. and Ross, J. Physical Chemistry, 2nd Edn., (Oxford, London, 2010).
5. Physical Chemistry. I. N. Levine, McGraw Hill.
6. Physical Chemistry. R. G. Mortimer, Academic Press.
7. Statistical Mechanics. D. A. McQuarrie, University Science Books.

B. SC. IN CHEMISTRY

DETAILED SYLLABUS OF FYUGP SEMESTER-VIII

Course Title: Advanced topics in Chemistry-I (DSC-19)

Course Code: MAJ-CHM-8.1

Total Credit: 4 (3 Credit Theory + 1 Credit Practical)

Distribution of marks: 70 (End Semester) (45T+25P) + 15 (In-Semester) + 15(HA/S/GD)

Course objective: The unit on reaction mechanism is included for the students to get acquainted with the oxidation reduction reaction, Outer-sphere and inner-sphere electron transfer reaction-characteristics and controlling factors, racemization in octahedral complexes etc. A course on transition metals in catalysis aims to equip students with a comprehensive understanding of how transition metals, with their unique properties, facilitate chemical reactions as catalysts, covering mechanisms, applications, and their role in both industrial and biological processes. The unit of Asymmetric synthesis is included to provide students with essential knowledge and practical skills in asymmetric synthesis. Further, students will be provided with advanced understanding to explore photochemical and fast reaction mechanisms, including energy transfer, quenching, reaction dynamics, and femtochemistry, with emphasis on theoretical models, molecular techniques, and their kinetic applications.

Theory: 3 Credits   Total course hour: 45 hr   Duration of Examination: 2 hr.

Unit 1: Inorganic Reaction Mechanism-II (10 Lectures)

Oxidation Reduction Reaction / Redox Reaction, Outer-sphere and inner-sphere electron transfer reaction-characteristics and controlling factors, ligand transfer, role of bridging ligand, chemical mechanism of electron transfer, complementary and non-complimentary redox reactions. racemization in octahedral complexes.

Unit 2: Transition metals in catalysis (10 Lectures)

Study of the following industrial processes and their mechanism:

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

Unit 3: Introduction to Asymmetric synthesis (10 Lectures)

Stereoselective and racemization reactions, Explanation of stereoselectivity using energy profile diagrams, Cram's Rule and Felkin-Anh model for predicting stereochemical outcomes, Use of chiral auxiliaries, chiral reagents, and chiral catalysts in asymmetric synthesis, Merits and demerits of chiral inducing agents, Evans oxazolidinones for enantioselective alkylation, Sharpless asymmetric epoxidation, CBS catalyst and its role in asymmetric reduction, Resolution of racemic mixtures via diastereomeric recrystallization and kinetic resolution, Asymmetric synthesis using the chiral pool approach, Mechanistic insights and efficiency of stereoselective transformations in organic synthesis.

Unit 4: Chemical Dynamics (15 Lectures)

Energy transfer in photochemical reactions: photosensitization and quenching, Stern-Volmer equation (quenching of fluoroscence), Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence, Oscillatory reactions.
Reaction in solutions, Bronsted-Bjerrum Equation, Unimolecular reactions, RRK, RRKM theory, molecular beam techniques, reaction dynamics, potential energy surface, Study of fast reactions, Femtochemistry.

Practical: 1 Credit Total course hour: 30 hr Duration of Examination: 3 hr

List of experiments:

(i) Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of analysis of constituents in three component mixtures, alloys and minerals.
(ii) Synthesis and characterization of inorganic compounds, including those involving green synthetic methodology: Characterization includes elemental analysis, studies by IR, electronic spectra, magnetic susceptibility, conductance measurements, cyclic voltammetry. TG, DSC.
(iii) Determine the rate constant of the acid catalyzed hydrolysis of methyl acetate.

(iv) Determine the rate constant of saponification of ethyl acetate.

(v) Determine the activation energy of the hydrolysis of methyl acetate catalyzed by hydrochloric acid.

Learning outcome:

On completion of this course the students will be able to understand:

(i) The students will be able to realise the role of crystal field theory and molecular orbital theory in controlling the reactivity of inorganic meal complexes.
(ii) The structures of industrially important different organometallic catalysts and details about their catalytic activities.
(iii) Students will grasp key concepts of asymmetric synthesis and stereoselective transformations.