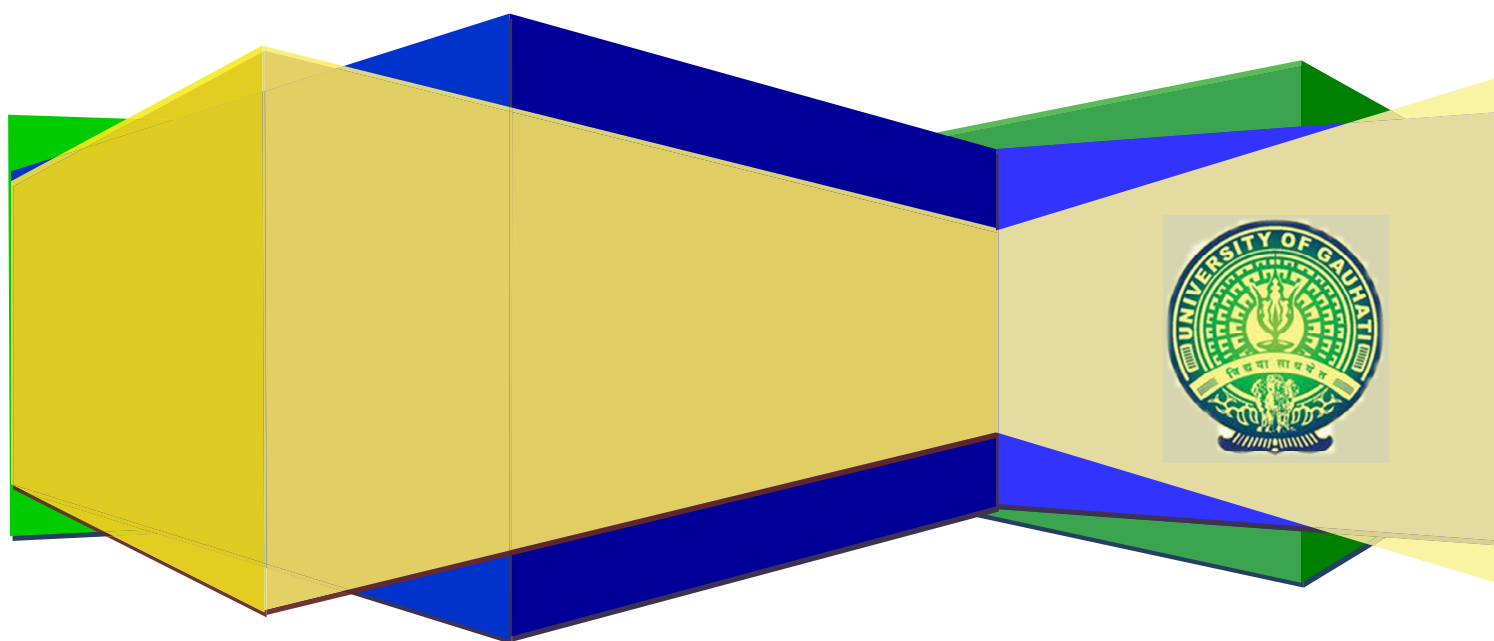


# Gauhati University

## Syllabus for FYUGP B.Sc. Chemistry



# Syllabus for B.Sc. FYUGP Chemistry



**Gauhati University**

Guwahati::Assam

**NEP –FYUGP**  
**Course Distribution**  
**Department of Chemistry**  
**Gauhati University**

| Department /Centre | Subject / Discipline | Course Title   | Semester   | Credit | Paper Type          |
|--------------------|----------------------|--|------------|--------|---------------------|
| Chemistry          | Chemistry            | Chemistry I  | Semester 1 | 4      | Compulsory          |
| Chemistry          | Chemistry            | Chemistry II   | Semester 2 | 4      | Compulsory          |
| Chemistry          | Chemistry            | Chemistry III  | Semester 3 | 4      | Compulsory          |
| Chemistry          | Chemistry            | Inorganic Chemistry - I                                    | Semester 4 | 4      | Compulsory          |
| Chemistry          | Chemistry            | Organic Chemistry - I                                      | Semester 4 | 4      | Compulsory          |
| Chemistry          | Chemistry            | Theoretical Chemistry                                      | Semester 4 | 4      | Compulsory/Elective |
| Chemistry          | Chemistry            | Magnetic Resonance Spectroscopy and Analytical Techniqiues | Semester 4 | 4      | Compulsory/Elective |
| Chemistry          | Chemistry            | Inorganic Chemistry-II                                     | Semester 5 | 4      | Compulsory/Elective |
| Chemistry          | Chemistry            | Organic Chemistry-II                                       | Semester 5 | 4      | Compulsory/Elective |
| Chemistry          | Chemistry            | Reaction Dynamics  | Semester 5 | 4      | Compulsory/Elective |
| Chemistry          | Chemistry            | Light-Matter Interaction                                   | Semester 5 | 4      | Compulsory          |
| Chemistry          | Chemistry            | Inorganic Chemistry - III                                  | Semester 6 | 4      | Compulsory/Elective |
| Chemistry          | Chemistry            | Organic Chemistry - III                                    | Semester 6 | 4      | Compulsory/Elective |
| Chemistry          | Chemistry            | Equllibria and Electrochemistry                            | Semester 6 | 4      | Compulsory/Elective |
| Chemistry          | Chemistry            | Industrial Chemistry                                       | Semester 6 | 4      | Compulsory          |

**Prerequisites:**

- For Major in Chemistry a student must pass in Chemistry and Mathematics at XII level.
- For Minor in Chemistry a student must pass in Chemistry at XII level.

## Semester-I: Chemistry I (3L- 0T-1P)

### Graduate Attributes

i. **Course Objective:**

This course aims at giving students insight into the fundamental aspects of atoms, ions and molecules in terms of their electronic structure and reactivity. Structure and bonding in/of these are to be dealt with basic quantum chemistry treatment. Further, periodic classification of elements to illustrate the changes in properties along the periods and groups to be emphasized upon. Properties of the gases and liquids are to be introduced.

Accompanying laboratory course is designed to introduce students to various laboratory apparatus, preparation of standard solutions, measurement of physical properties, and laboratory safety.

ii. **Learning outcome:**

On successful completion, students would have clear understanding of the concepts related to atomic and molecular structure, chemical bonding, periodicity and states of matter. Students will be able to work in a chemical laboratory following standard safety protocols.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Dr. Sonit Kumar Gogoi, Gauhati University, skgogoi@gauhati.ac.in

2) Dr. Dhriti Mahanta, Gauhati University, mdhriti@gauhati.ac.in



**Semester-I: Chemistry I (3L- 0T-1P)**

| <b>Unit</b>   | <b>Content</b>  | <b>Contact Hours</b> |
|---|---|----------------------|
| Unit I:<br>Atomic structure                         | Historical development on structure of atom; Bohr's model, H-atom spectrum; black body radiation; photoelectric effect (qualitative treatment only); The dual behaviour and uncertainty. Quantum mechanical approach to atomic structure: concept of wave function, well behaved function, operator, normalised and orthogonal wave function, Schrodinger wave equation, eigenfunction, Significance of $\Psi$ and $\Psi^2$ , Particle in a 1-D box; Schrodinger equation of hydrogen atom (no derivation), radial and angular wave functions for hydrogen atom, probability distribution, quantum numbers, Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations. | 8                    |
| Unit II:<br>Periodicity and chemical behaviour      | Effective nuclear charge; Slater's Rule; covalent and ionic radii, ionization energies, electronegativity (various scales), electron affinities   | 3                    |
| Unit III:<br>Chemical bonding I (ionic interaction) | General characteristics of ionic compounds; lattice and solvation energy; Born Lande equation; Kapustinski equation, Madelung constant, Born Haber cycle for lattice energy calculation   | 4                    |
| Unit IV:<br>Structure of organic molecules          | Nature of bonding: hybridisation of atomic orbitals (qualitative VB and MO approach); effect of hybridization on bond properties.   | 4                    |
| Unit V:<br>Stereochemistry of organic molecules     | Representation of organic molecules in 2D and 3D (Fischer, Newman and Sawhorse projection formulae and their interconversions); geometrical isomerism (cis-trans, syn-anti, E/Z notations); concept of chirality (enantiomers and diastereomers); configuration and conformation, barriers to rotation, conformational analysis (ethane, butane, cyclohexane)   | 8                    |
| Unit VI:<br>Electronic effects in organic molecules | Concept of electrophiles and nucleophiles; inductive effects; resonance, conjugation and delocalisation.  | 3                    |

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| Unit VII:<br>Gaseous<br>state | Causes of deviation from ideal gas behaviour, compressibility factor, $Z$ , and its variation with pressure and temperature for different gases. State variables and equation of states for real gases; van der Waals equation of state, its derivation and application in explaining real gas behaviour. Reasons and examples of failure of van der Waal equation of state and interpretation of van der Waals pressure-volume isotherm. Critical state and phenomena, mathematical definition and interpretation of critical point, relation between critical constants and van der Waals constants: along with their thermodynamic interpretation. Introduction to virial equation and virial coefficients, derivation of Boyle temperature. | 8 |
| Unit VIII:<br>Liquid<br>state | Qualitative treatment of the structure of the liquid state. Physical properties of liquids: vapour pressure, surface tension coefficient of viscosity, and their determination. Temperature variation of viscosity of liquids and comparison with that of gases. Effect of addition of various solutes on surface tension and viscosity. Explanation of cleansing action of detergents (micelle formation and critical micelle concentration).  | 7 |

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| <p>Laboratory Course I</p> | <p>1. Introduction to laboratory apparatus and safety measures in laboratory,<br/> 2. Calibration of apparatus (volumetric flask, thermometer, melting point apparatus etc.)</p> <p><b>Group A</b><br/> (a) Preparation of normal and molar solution, for example KCl, Na<sub>2</sub>C<sub>2</sub>O<sub>4</sub>, HCl, H<sub>2</sub>SO<sub>4</sub> etc. (Verification by conductometric measurement).<br/> (b) Determination of solubility of a given salt at different temperature and plot solubility curve.<br/> (c) Determination of water of crystallisation of hydrated salt by ignition and weighing.</p> <p><b>Group B</b><br/> (a) Determination of the melting points of organic compounds (here, the student is required to learn about thermometer calibration before performing the experiment).<br/> (b) Effect of impurities on the melting point – mixed melting point of two unknown organic compounds.<br/> (c) Purification of organic compounds by crystallization using the following solvents: (a) water, (b) alcohol, (c) alcohol-water mixture.</p> <p><b>Group C</b><br/> (a) Evaluating the compressibility factor using standard packages such as Excel/Origin/Python/Fortran.<br/> (b) Simulating an ideal gas using programming.<br/> (c) Simulation of a real gas using programming.<br/> (d) To determine the partial molar volume of ethanol-water mixture at a given composition.<br/> (e) Determine the surface tension of a given liquid at room temperature using stalagmometer by drop number method.<br/> (f) Determine the surface tension of a given liquid by means of stalagmometer using drop weight method.<br/> (g) Determine the composition of a given mixture by surface tension method.<br/> (h) Study the variation of surface tension of detergent solutions with concentration.</p> <p><i>(Students are required to perform Exp. 1, 2 and a minimum of two experiments from each group)</i></p> | <p>30</p> |
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|---------------------------|---|
| Text Book /Reference Book | <ol style="list-style-type: none"> <li>1. University Chemistry, P. Siska, O. K. Medhi, 2<sup>nd</sup> edition, Pearson Education</li> <li>2. General and Inorganic Chemistry, R.P. Sarkar (part 1) 3<sup>rd</sup> edition, NCBA</li> <li>3. Concise Inorganic Chemistry, J. D. Lee, 5<sup>th</sup> Edition, Pearson Education</li> <li>4. Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5<sup>th</sup> edition, Pearson Education</li> <li>5. Principles of Physical Chemistry, Puri, Sharma, Pathania, 48<sup>th</sup> Edition, Vishal Publishing Com.</li> <li>6. Atkins Physical Chemistry, Atkins, de Paula and Keeler, 11<sup>th</sup> Edition, Oxford University Press.</li> <li>7. Stereochemistry of Organic Compounds, D. Nasipuri, 4<sup>th</sup> Edition.</li> <li>8. Reaction Mechanism in Organic Chemistry, S. M. Mukherji, S. P. Singh, 3<sup>rd</sup> Edition.</li> <li>9. Organic Reactions and their Mechanisms, P. S. Kalsi, 5<sup>th</sup> Edition.<br/>Solomons' Organic Chemistry, T. W. G. Solomons, C. B. Fryhle, S. A. Snyder.</li> </ol> |
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## Semester-II: Chemistry II (3L- 0T-1P)

### Graduate Attributes

i. **Course Objective:**

This course extends the concepts of chemical bonding and introduces to coordination chemistry. The students will be familiarized with the organic reactive intermediates. Elementary concepts of acidity, basicity and thermodynamics are to be deliberated. Laboratory experiments relevant to the topics in the theory are included for the students to appreciate the concepts and to hone the experimental skills.

ii. **Learning outcome:**

Students shall understand and apply the concepts of chemical bonding, coordination chemistry, acids and bases and the reactive intermediates. They shall also understand the chemistry from a thermodynamic point of view. Students will acquire preliminary training on quantitative analysis, synthesis of coordination compounds, qualitative analysis of organic compounds and measurement of a few basic thermodynamic parameters.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Prof. Anup Kumar Talukdar, Gauhati University, aktalukdar@gauhati.ac.in

2) Dr. Arabinda Baruah, Gauhati University, arb@gauhati.ac.in

**Semester-II: Chemistry-II (3L- 0T-1P)**

|   |   |    |
|---|---|----|
| Unit I:<br>Chemical bonding (covalent bond and chemical forces) | Valence bond theory (Heitler-London approach), energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, resonance and resonance energy, molecular orbital theory (MOT). Molecular orbital diagrams of homonuclear ( $N_2$ , $O_2$ ) and heteronuclear diatomic ( $CO$ , $NO$ , $CN^-$ ), bonding in $BeF_2$ and $HCl$ (idea of s-p mixing and orbital interaction). Valence shell electron pair repulsion theory (VSEPR). Covalent character in ionic compounds, polarising power and polarizability. Fajan's rules and consequences of polarisation. Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.<br>Weak chemical forces (van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, instantaneous dipole-induced dipole interactions and hydrogen bonding) and their effects on melting and boiling points, solubility and hydration energy. | 10 |
| Unit II:<br>Coordination chemistry-I (structure and isomerism)  | Introduction to coordination complexes (Werner theory, types of ligands) IUPAC nomenclature, isomerism in coordination complexes, stereochemistry of complexes with coordination numbers 4, 5, and 6. Berry pseudorotation.   | 5  |
| Unit III:<br>Reactive intermediates in organic reactions        | Formation, structure and stability of reactive intermediates: carbocations, carbanions, radicals, carbenes, nitrenes, benzyne (brief mechanistic perspective using concepts of substitution, addition, elimination and rearrangements reactions).   | 12 |
| Unit IV:<br>Acidity, basicity, and $pK_a$                       | The definition of $pK_a$ ; Lewis acids and bases; organic acids and bases (factors affecting relative strength); substituents affect the $pK_a$ (carbon acids).   | 3  |

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| <p>Unit V:<br/>Thermodynamics</p> | <p>Mathematical treatment: exact and inexact differentials, partial derivatives, Euler's reciprocity, cyclic rules.</p> <p>Intensive and extensive variables. Isolated, closed and open systems. Cyclic, reversible and irreversible processes. Zeroth law of thermodynamics. First law of thermodynamics, concept of heat (q) and work (w), internal energy(U) and enthalpy (H) in differential forms: their molecular interpretation. Calculation of w, q, <math>\Delta U</math> and <math>\Delta H</math> for expansion of ideal gas under isothermal and adiabatic conditions for reversible and irreversible processes. Derivation of Joule-Thomson coefficient and inversion temperature.</p> <p>Application of first law of thermodynamics: standard state, standard enthalpy changes of physical and chemical transformations: fusion, sublimation, vaporization, solution, dilution, neutralization, ionization. Bond-dissociation energy Kirchhoff's equation, relation between <math>\Delta H</math> and <math>\Delta U</math> of a reaction. Difference between enthalpy and standard enthalpy.</p> <p>Second law of thermodynamics, entropy (S) as a state function, molecular interpretation of entropy. Residual Entropy. Free energy: Gibbs function (G) and Helmholtz function (A) and their molecular interpretation. Difference between free energy and standard free energy. Gibbs-Helmholtz equation, criteria for thermodynamic equilibrium and spontaneity of a process. Maxwell's Relations and their physical significance.</p> | <p>15</p> |
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| Laboratory Course II      | <p>1. Preparation of buffer solution and measurement of pH using pH-meter (acetic acid-sodium acetate buffer)</p> <p><b>Group A:</b></p> <p>(a) Determination of total hardness of water by titration against standardised EDTA solution.</p> <p>(b) Synthesis of coordination compounds</p> <ol style="list-style-type: none"> <li>i) Potassium tris(oxalato)chromate(III),</li> <li>ii) [Ni(DMG)<sub>2</sub>]</li> </ol> <p><b>Group B:</b></p> <p>(a) Qualitative organic analysis for N, S and halogen in a given organic compounds.</p> <p>(b) Detection of presence of unsaturation and aromaticity in an organic sample.</p> <p>(c) Identify acidic functional groups of a given organic sample (Acetic acid, Lactic acid, Tartaric acid and Phthalic acid) and determine the pK<sub>a</sub> by titrimetric methods.</p> <p><b>Group C:</b></p> <p>(a) Determination of heat capacity of a calorimeter and enthalpy of neutralisation (eg. hydrochloric acid with sodium hydroxide).</p> <p>(b) Determine the enthalpy of solution of oxalic acid from solubility measurements.</p> <p>(c) Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).</p> <p>(d) Calculation of ionization enthalpy of ethanoic acid.</p> <p>(e) Determination of enthalpy of hydration of copper sulphate.</p> <p><i>(Students are required to perform Exp. 1 and minimum of two from each group)</i></p> | 30 |
| Text Book /Reference Book | <ol style="list-style-type: none"> <li>1. General and Inorganic Chemistry, R.P. Sarkar (part 1) 3<sup>rd</sup> edition, NCBA</li> <li>2. Concise Coordination Chemistry, R. Gopalan, V. Ramalingam, 1<sup>st</sup> edition, Vikash Publishing House</li> <li>3. Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5<sup>th</sup> edition, Pearson Education</li> <li>4. Principles of Physical Chemistry, Puri, Sharma, Pathania, 48<sup>th</sup> edition, Vishal Publishing Com.</li> <li>5. Atkins Physical Chemistry, Atkins, de Paula and Keeler, 11<sup>th</sup> edition, Oxford University Press.</li> <li>6. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith 7<sup>th</sup> edition (Wiley).</li> <li>7. Organic Chemistry, G. M. Loudon, 4<sup>th</sup> edition.</li> <li>8. Mechanism and Theory in Organic Chemistry, Sachin Kumar Ghosh, New Central Book Agency.</li> </ol>  |    |



## Semester-III: Chemistry III (3L- 0T-1P)

### Graduate Attributes

i. **Course Objective:**

This course extends the concepts of acids/bases and coordination chemistry as well as gives introductions to the redox reactions, ideal solutions and colligative properties. Further, the course is intended to apprise students about different classes of organic compounds, such as halogenated hydrocarbons, alcohols, phenols, thiols, epoxides and carbonyls.

Through the accompanying laboratory experiments on volumetric analysis, identification and preparation of derivatives and determination of physical properties of liquids, this course intends to make students learn about the qualitative and quantitative aspects of the analysis.

ii. **Learning outcome:**

On successful completion of the course students will have significant knowledge of acids/bases as well as an overview of bonding in coordination compounds, principles of redox chemistry, solutions and their properties. Students will also be able to describe and classify organic compounds in terms of their functional groups and reactivity. Further experiments on acid/base and redox titrations will enable the students to consolidate their skills on quantitative analysis. In addition, qualitative analysis of organic compounds having common functional groups will give the students an idea about functional groups and their reactivities. Physical chemistry experiments will introduce the students to physical property measurements and kinetics of chemical reactions.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Dr. Sanfaori Brahma, Gauhati University, sanfaori@gauhati.ac.in

2) Dr. Tridib Kumar Goswami, Gauhati University, tridib@gauhati.ac.in

**Semester III: Chemistry-III (3 L-0 T-1 P)**

| <b>Unit</b>  | <b>Content</b>   | <b>Contact Hrs</b> |
|--|--|--------------------|
| Unit I: Acid and Bases                                   | Acid-base concepts, measure of acid and base strength, proton affinity, acidity and basicity of binary hydrogen compounds, inductive effect and strength of oxyacids, acidity of aqua ions, steric effect, proton sponge, solvation and acid base strength, non-aqueous solvents and acid base strength, levelling effect, superacids and superbases. Hard and soft acids and bases (HSAB), application of HSAB principle and symbiosis. | 7                  |
| Unit II: Oxidation and reduction -I                      | Reduction potentials: Redox half-reactions, standard potentials and spontaneity, trends in standard potentials, the electrochemical series, Nernst equation (Influence of pH and concentration on electrode potential). Principles of redox titration and choice of redox indicators.  | 4                  |
| Unit III: Coordination chemistry-II                      | Valence bond theory (VBT), inner and outer orbital complexes, electroneutrality principle and back bonding, effects of hybridization in metal ligand bond strength and stability of complexes, choice of metal d-orbital(s) in hybridization in different coordination geometries, magnetic properties of complexes, drawback of VBT.  | 4                  |
| Unit IV: Aromaticity                                     | Concepts of aromatic, anti-aromatic and non-aromatic compounds (including examples of cyclic carbocations, carbanions and heterocyclic compounds); Hückel's rule.  | 3                  |
| Unit V: Hydrocarbons and halogenated compounds           | Methods of preparation, properties and relative reactivity of alkyl and aryl halides; Selectivity in electrophilic and nucleophilic substitution reactions ( $S_NAr$ ), Preparation and reactions of diazonium salts; Benzyne mechanism.   | 4                  |
| Unit VI: Alcohols, phenols, thiols and related compounds | Preparation, properties and relative reactivity of 1°, 2°, and 3°-alcohols, ethers, epoxides (preparation and reactions with alcohols, ammonia derivatives and $LiAlH_4$ ). Thiols and sulfides; phenols (preparation, properties and reactivity; Reimer-Tiemann and Kolbe's-Schmidt Reactions)  | 4                  |
| Unit VII: Carbonyl compounds                             | Structure, reactivity and preparation; oxidations and reductions (Jones reagent, PCC and PDC, Oppenauer, Clemmensen, Wolff-Kishner, $NaBH_4$ , $LiAlH_4$ , MPV), Baeyer Villiger oxidation.  | 4                  |

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| Unit VIII:<br>Solution               | Vapour pressure of solution. Ideal solutions, ideally diluted solutions and colligative properties. Raoult's law & Henry's Law. Thermodynamic derivation of colligative properties of solution (using chemical potentials) and their inter-relationships. Abnormal colligative properties.   | 7  |
| Unit IX:<br>Partial molar quantities | Fugacity, activity coefficients and concept of chemical potential: Gibbs Duhem equation and Duhem-Margules equation: their use and application, Enthalpy, free energy and entropy of mixing, excess thermodynamic functions.   | 8  |
| Laboratory Course III                | <p><b>Group A</b></p> <p>(a) Acid-base titration: estimation of carbonate, bicarbonate and hydroxide.</p> <p>(b) Redox titration: estimation of Fe(II) using standardised <math>\text{KMnO}_4</math> solution.</p> <p>(c) Determination of water of crystallisation of Mohr Salt using standardised <math>\text{KMnO}_4</math> solution.</p> <p>(d) Estimation of Fe(II) with <math>\text{K}_2\text{Cr}_2\text{O}_7</math> using internal indicator (diphenylamine).</p> <p><b>Group B</b></p> <p>(a) Identification of functional groups in a given organic sample: Simple functional groups such as alcohols, phenols, amines, nitro, carbonyl and carboxylic acid groups.</p> <p>(b) Prepare derivatives of a given organic sample containing single functional group (i.e. alcohols, phenols, amines, nitro, carbonyl and carboxylic acid group).</p> <p><b>Group C</b></p> <p>(a) Determine the surface tension of a given solution at room temperature using a stalagmometer.</p> <p>(b) Determine the viscosity of a liquid at a given concentration at laboratory temperature, by viscometer.</p> <p>(c) Determine the composition of a given liquid mixture by viscosity method.</p> <p>(d) Study the variation of viscosity of sucrose solution with the concentration of the solute.</p> <p>(e) Compare the strengths of HCl and <math>\text{H}_2\text{SO}_4</math> by studying kinetics of hydrolysis of methylacetate.</p> <p><i>(Students need to perform at least three experiments from Group A and C. Group B is compulsory.)</i></p> | 30 |

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| Text/ Reference Books: | <ol style="list-style-type: none"> <li>1. General and Inorganic Chemistry, R.P. Sarkar (part 1), 3<sup>rd</sup> edition, NCBA.</li> <li>2. Concise Coordination Chemistry, R. Gopalan, V. Ramalingam, 1<sup>st</sup> edition, Vikash Publishing House.</li> <li>3. Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5<sup>th</sup> edition, Pearson Education.</li> <li>4. Principles of Physical Chemistry, Puri, Sharma, Pathania, 48<sup>th</sup> edition, Vishal Publishing House.</li> <li>5. Atkins Physical Chemistry, Atkins, de Paula and Keeler, 11<sup>th</sup> edition, Oxford University Press.</li> <li>6. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith 7<sup>th</sup> edition (Wiley).</li> <li>7. Organic Chemistry, Volume 1, I. L. Finar, 5<sup>th</sup> edition.</li> <li>8. Organic Chemistry, L. G. Wade Jr., Maya Shankar Singh, 6<sup>th</sup> edition.</li> <li>9. Organic Chemistry, P. Y. Bruice, 8<sup>th</sup> edition, Pearson Education.</li> </ol> |  |
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## Semester—IV: Inorganic Chemistry-I (3L -0T-1P)

### Graduate Attributes

i. **Course Objective:**

This course aims at giving an introduction to molecular symmetry, *d*-block chemistry, metallurgy, lanthanides, actinides and nuclear chemistry while extending the concepts of coordination and redox chemistry.

Qualitative inorganic analysis is included to give students practical experience on applications of inorganic chemistry. Students should learn how differential reactivity under different conditions of pH can be used to identify variety of ions in a complex mixture.

ii. **Learning outcome:**

On successful completion the students will be able to assign the point groups of molecules, explain bonding in coordination compounds, explain their various properties in terms of CFSE and predict reactivity.

Students will have an overview of the metallurgical and nuclear processes as well as the chemistry of *d* and *f*-block elements.

Students in general will learn the use of concepts like solubility product, common ion effect, pH etc. in the analysis of ions. They will also appreciate how a clever design of reactions makes it possible to identify the components in a mixture.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Dr. Saitanya Bharadwaj, Pragjyotish College, [saitanya.iitg@gmail.com](mailto:saitanya.iitg@gmail.com)

2) Dr. Sonit Kumar Gogoi, Gauhati University, [skgogoi@gauhati.ac.in](mailto:skgogoi@gauhati.ac.in)

**Semester –IV, Inorganic Chemistry-I (3L -0T-1P)**

| <b>Unit</b>                                   | <b>Content</b>   | <b>Contact Hours</b> |
|---|--|----------------------|
| Unit I:<br>Introduction to molecular symmetry | Symmetry elements and operations, molecular point groups, symmetry elements present in $C_{2v}$ , $C_{3v}$ , $T_d$ and $O_h$ point group (pictorial representation), introductory idea of character tables, Mulliken symbols.  | 6                    |
| Unit II: d-block Chemistry                    | Chemistry of first row transition elements (Ti-Cu) in various oxidation states as halides and oxides, comparison of the first, second and third transition series elements.  | 8                    |
| Unit III<br>Coordination chemistry III        | Crystal Field Theory (CFT) (qualitative treatment): d-orbital splitting in tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral geometries, calculation of CFSE, thermodynamic and structural aspect of orbital splitting, pairing energies (contribution of exchange and coulomb energy), factors affecting the magnitude of $10 Dq$ ( $\Delta_o$ , $\Delta_t$ ), spectrochemical series, tetragonal distortions from octahedral geometry and Jahn-Teller theorem. Limitations of CFT (nephelauxetic effect and EPR evidences), Elementary idea on ligand field theory, molecular orbital theory (MOT) with special reference to sigma bonded octahedral and tetrahedral complexes (qualitative treatment only), pi bonding in octahedral complexes. Metal-metal quadruple bond in $[Re_2Cl_8]^{2-}$ . | 10                   |
| Unit IV:<br>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 agents. Electrolytic reduction, methods of purification of metals: electrolytic Kroll process, Parting process, van Arkel-de Boer process and Mond's process, Zone refining.   | 5                    |
| Unit V:<br>Oxidation and reduction -II        | Redox stability: reaction with water, oxidation by atmospheric oxygen, disproportionation and comproportionation, the influence of complexation, relation between solubility and standard potential.<br>Diagrammatic representation of potential data (Latimer diagram, Frost diagram, Pourbaix diagram).  | 6                    |
| Unit VI:<br>Lanthanoids and Actinoids         | Lanthanoids: electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only). Coordination chemistry of lanthanides.<br>Actinoids: electronic configuration, oxidation states, magnetic properties, comparison with lanthanides.  | 6                    |

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|--|--|----|
| Unit VII:<br>Nuclear<br>Chemistry                          | Stability of nucleus and radioactive decay processes, Fermi theory, half-lives, Auger effect, Mass defect, Nuclear reactions – notations, comparison with chemical reaction: Types of nuclear reactions. Applications of radioisotopes in age determination.   | 4  |
| <b>Laboratory:</b><br>Inorganic<br>Qualitative<br>Analysis | Qualitative analysis of mixtures containing four cations and anions. Emphasis should be given to the understanding of reactions. The following radicals are suggested: $\text{CO}_3^{2-}$ , $\text{NO}_2^-$ , $\text{S}^{2-}$ , $\text{SO}_3^{2-}$ , $\text{S}_2\text{O}_3^{2-}$ , $\text{CH}_3\text{COO}^-$ , $\text{F}^-$ , $\text{Cl}^-$ , $\text{Br}^-$ , $\text{I}^-$ , $\text{NO}_3^-$ , $\text{BO}_3^{3-}$ , $\text{C}_2\text{O}_4^{2-}$ , $\text{PO}_4^{3-}$ , $\text{NH}_4^+$ , $\text{K}^+$ , $\text{Pb}^{2+}$ , $\text{Cu}^{2+}$ , $\text{Cd}^{2+}$ , $\text{Bi}^{3+}$ , $\text{Sn}^{2+}$ , $\text{Sb}^{3+}$ , $\text{Fe}^{3+}$ , $\text{Al}^{3+}$ , $\text{Cr}^{3+}$ , $\text{Zn}^{2+}$ , $\text{Mn}^{2+}$ , $\text{Co}^{2+}$ , $\text{Ni}^{2+}$ , $\text{Ba}^{2+}$ , $\text{Sr}^{2+}$ , $\text{Ca}^{2+}$ , $\text{Mg}^{2+}$<br>Mixtures should preferably contain one interfering anion, or insoluble component ( $\text{BaSO}_4$ , $\text{SrSO}_4$ , $\text{PbSO}_4$ , $\text{CaF}_2$ or $\text{Al}_2\text{O}_3$ ) or combination of anions such as $\text{CO}_3^{2-}$ and $\text{SO}_3^{2-}$ , $\text{NO}_2^-$ and $\text{NO}_3^-$ , $\text{Cl}^-$ and $\text{Br}^-$ , $\text{Cl}^-$ and $\text{I}^-$ , $\text{Br}^-$ and $\text{I}^-$ , $\text{NO}_3^-$ and $\text{Br}^-$ , $\text{NO}_3^-$ and $\text{I}^-$ .<br>Spot tests should be done whenever possible. | 30 |
| Text Books/<br>Reference<br>Books                          | <ol style="list-style-type: none"> <li>1. Inorganic Chemistry, G.L. Meissler and D. A. Tarr, 5<sup>th</sup> edition, Pearson.</li> <li>2. Inorganic Chemistry, P. Atkins, Overtone Rourke, Weller and Armstrong 5<sup>th</sup> edition, Oxford.</li> <li>3. Principles of Inorganic Chemistry, 7<sup>th</sup> edition, Puri, Sharma, Kalia, Vishal Publishing Co.</li> <li>4. Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5<sup>th</sup> edition, Pearson Education.</li> <li>5. Advanced Inorganic Chemistry, F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Murillo, Manfred Bochmann, Wiley.</li> <li>6. Vogel's Qualitative Inorganic Analysis, 7<sup>th</sup> Edition, G. Svehla, B Sivasankar, Pearson.</li> </ol>   |    |

## Semester-IV: Organic Chemistry I (3 L- 0 T- 1 P)

### Graduate Attributes

i. **Course Objective:**

The objective of this course is to illustrate the structure and reactivity of organic compounds containing carboxylic acid/derivatives, nitrogen-based functional groups as well as heterocyclic compounds. Students will apply these basic concepts towards the understanding of amino acids, peptides/proteins and alkaloids.

Experiments are designed to familiarize the students with organic synthesis and purification.

ii. **Learning outcome:**

On successful completion students will be able to explain and correlate the structure and reactivity of oxygen and nitrogen containing organic molecules having relevance to bioorganic systems. Students will be able to perform simple organic transformations and purifications following conventional/green pathways.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Prof. Rupam Jyoti Sarma, Gauhati University, rjs@gauhati.ac.in

2) Dr. Ranjit Thakuria, Gauhati University, ranjit.thakuria@gauhati.ac.in



**Semester-IV: Organic Chemistry I (3 L- 0 T- 1 P)**

| <b>Unit</b>                                    | <b>Content</b>   | <b>Contact Hours</b> |
|--|--|----------------------|
| Unit I: Carboxylic acids and their derivatives | Preparation, properties and reactions of carboxylic acids: reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids.<br>Preparation and reactions of acid chlorides, anhydrides, esters and amides; comparison of nucleophilic substitution at acyl group: mechanism of acidic and alkaline hydrolysis of esters; Claisen condensation, Dieckmann and Reformatsky reactions. | 10                   |
| Unit II: Nitrogen containing functional groups | Preparation and properties of amines: effect of substituent and solvent on basicity; Gabriel phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hofmann-elimination reaction; distinction between 1°, 2° and 3° amines with Hinsberg reagent and nitrous acid. Diazonium Salts: preparation and their synthetic applications.<br>General methods for preparation of nitro compounds, nitriles and isonitriles and important reactions.                     | 8                    |
| Unit III: Amino acids, peptides and proteins   | $\alpha$ -Amino acids (synthesis and reactions); zwitterions, pK <sub>a</sub> values, isoelectric point and electrophoresis; structure of the peptide bond; primary, secondary and tertiary structures of proteins; intramolecular interactions in protein binding site; mechanism of enzyme action (acid-base catalysis); enolization reactions; thioesters; enzyme inhibitors; determination of peptide sequence.  | 7                    |
| Unit IV: Heterocyclic compounds                | Classification and nomenclature (5-numbered and 6-membered rings with one heteroatom); synthesis and reactions of furan, pyrrole, thiophene, pyridine and indoles: selected name reactions (Paal-Knorr synthesis, Knorr synthesis, Hantzsch synthesis, Fischer indole synthesis, Madelung synthesis)   | 7                    |
| Unit V: Alkaloids                              | Natural occurrence, general structural features, isolation and their physiological action; Hoffmann's exhaustive methylation, Emde's modification, structure elucidation of nicotine; medicinal importance of nicotine, hygrine, quinine, morphine and cocaine.  | 6                    |
| Unit VI: Organic spectroscopy                  | Introduction to UV-visible and infrared spectroscopy in structure elucidation of organic compounds; relation between absorption spectroscopy and molecules containing conjugated C=C and C=O groups; analysis of compounds containing alkenes, alkynes and carbonyl compounds using infrared spectroscopy (conceptual aspects).  | 7                    |

|                   |   |    |
|-------------------|---|----|
| Laboratory Course | <p>1. Organic preparations (any two from each): benzylation of organic compounds: amines (aniline, toluidines, anisidine) and phenols (phenol, <math>\beta</math>-naphthol, salicylic acid) by the following methods:<br/>           (i) Using conventional method.<br/>           (ii) Using green chemical approach.</p> <p>2. Organic preparations (any three):<br/>           (i) Bromination of acetanilide by conventional methods.<br/>           (ii) Nitration of salicylic acid using ceric ammonium (green chemistry approach).<br/>           (iii) Selective reduction of <i>m</i>-dinitrobenzene to <i>m</i>-nitroaniline<br/>           (iv) Oxidation of ethanol/ isopropanol (iodoform reaction).<br/>           (v) Aldol condensation using either conventional or green method.<br/>           (vi) Benzil-Benzilic acid rearrangement.</p> <p>3. Chromatography: (a) Separation of a mixture of two amino acids by ascending paper chromatography; (b) Separation of a mixture of <i>o</i>- and <i>p</i>-nitrophenol or <i>o</i>- and <i>p</i>-nitroaniline by thin layer chromatography (TLC).</p>                  | 30 |
| Recommended books | <ol style="list-style-type: none"> <li>1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith 7<sup>th</sup> Edition.</li> <li>2. Organic Chemistry, Jonathan Clayden, Nick Greeves, Stuart Warren, 2<sup>nd</sup> Edition.</li> <li>3. Principles of Organic Synthesis, R. O. C. Norman, J. M. Coxon, 3<sup>rd</sup> Edition.</li> <li>4. Organic Chemistry, P. Y. Bruice, 8<sup>th</sup> Edition.</li> <li>5. Organic Chemistry, Volume 2, I. L. Finar, 5<sup>th</sup> Edition.</li> <li>6. Organic Chemistry, P. Y. Bruice, 8<sup>th</sup> Edition.</li> <li>7. Organic Spectroscopy, 3<sup>rd</sup> Edition, William Kemp.</li> <li>8. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampman, G. S. Kriz, 4<sup>th</sup> Edition.</li> <li>9. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, Pearson, 2012.</li> <li>10. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press.</li> <li>11. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3<sup>rd</sup> Edition Longman, 1978.</li> </ol> |    |

## Semester-IV: Theoretical Chemistry (3L-0T-1P)

### Graduate Attributes

i. **Course Objective:**

The aim of this course is to introduce the students to the important areas of quantum chemistry. Laboratory experiments are designed to give the students an insight into the different programming languages such as BASIC, FORTRAN, Python and their applications in calculation of physical properties.

ii. **Learning outcome:**

Students shall understand the fundamentals of atomic structure and its relation to quantum mechanics. They will be able to formulate the basic structural properties of atoms in terms of mathematical theories. Students shall be able to plot, and program equations related to simple chemical systems using computers.

Students shall be solving chemical problems using complex mathematics. This will develop a critical thinking ability to treat simple systems.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Dr. Himangshu Prabal Goswami, Gauhati University, hpg@gauhati.ac.in

2) Dr. Dhruba Jyoti Kalita, Gauhati University, dhrubajyoti.kalita@gauhati.ac.in

**Semester IV - Theoretical Chemistry (3L-0T-1P)**

| Unit   | Content   | Contact Hrs |
|--|---|-------------|
| Unit I:<br>Quantum Theory  | <p>Planck's Quantization of energy and Hydrogen Line spectrum. Postulates of quantum mechanics and their physical interpretation, wavefunctions and quantum mechanical operators. Born interpretation. Well behaved wavefunctions and commutation relations. Orthonormality and physical meaning of expanding a wavefunction in orthonormal basis. Hermitian Operators and Real Eigenvalues, Eigenvectors: their physical significance.</p> <p>Particle in a 1-D box (complete solution with orthonormalization) and relation to conjugated polyenes. Heisenberg Uncertainty Principle from expectation values of 1 D box, extension to two and three-dimensional boxes. Qualitative idea of tunneling.</p> <p>Rotational Motion and Energy: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels.</p> <p>Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels. Interpretation of zero-point energy.</p> <p>Hamiltonian for 1 electron H-atom, its wavefunctions (only explanation, no derivation) and its relation to atomic orbitals. Constructing Radial and Angular Distribution Curves from H-like wave functions. Quantum mechanical idea of chemical bond formation: Heitler-London's Valence bond theory. Atomic Units. Good quantum numbers for multi-electron systems and Atomic Term Symbols. LS and j-j coupling schemes.</p> | 37          |
| Unit II:<br>Molecular Properties                                 | Intermolecular forces and potentials. Polarizability of atoms and molecules, dielectric constant and polarisation, molar polarisation for polar and non-polar molecules. Clausius-Mosotti equation (with derivation) and Debye equations: their applications.   | 8           |
| Laboratory experiments (Minimum of seven experiments to be done) | <ol style="list-style-type: none"><li>1. Writing and plotting basic expressions and corresponding graphs (eg. Maxwell-Boltzmann distribution law, radial and angular distribution functions for H-atom etc.) using any spreadsheet software such as MS Excel/LibreOffice etc or simple programming language (GWBasic, FORTRAN, python etc)</li><li>2. Plotting the wavefunction and the energy expressions for particle in a box for <math>n = 1, 2</math> and <math>3</math> using any spreadsheet software such as MS Excel/LibreOffice etc or simple programming language (GWBasic, FORTRAN, python etc).</li><li>3. Numerical evaluation of the expectation values of position and square of momentum for particle in a 1 D box using the definition of the wavefunction and expectation value using any spreadsheet software such as MS Excel/LibreOffice etc or simple programming language (GWBasic, FORTRAN, python etc).</li><li>4. Plotting simple one-dimensional intermolecular potential energies (eg. harmonic, anharmonic, Lennard-Jones potential etc)</li></ol>  | 30          |

using any spreadsheet software such as MSExcel/LibreOffice etc or simple programming language (GWBasic, FORTRAN, python etc) and interpreting the potentials.

5. Numerical solution of the 1D Schrodinger equation for particle in a box using any spreadsheet software such as MSExcel/LibreOffice etc or simple programming language (GWBasic, FORTRAN, python etc).

6. Numerical solution of the 1D Schrodinger equation for particle in a box (with constant nonzero potential,  $V$ ) using any spreadsheet software such as MSExcel/LibreOffice etc or simple programming language (GWBasic, FORTRAN, python etc) and understand the role of  $V$  on the energy and wavefunction.

7. Geometry optimization (energy minimization): Making input file through selection of simple calculation method (e.g., STO/GTO, Hartree Fock or Density Functional Theory), basis set, specifying charge and multiplicity using any quantum chemistry software.

8. Frequency calculation: Locating results in output file, displaying calculated properties through molecular viewing software such as Avogadro, MacMolPlt, VMD, GaussView.

9. Calculation of the energy of the H-like atoms (H, He<sup>+</sup> etc) using the simple theoretical methods and simple basis sets. Tabulate the energy (in Hartree) and number of basis functions for each calculation.

10. Comparison of energy results with the exact value and discussing the effect of the number of basis functions and the discussion of the effect of increasing nuclear charge on the energy.

11. Performing optimization of simple organic molecules (like malonaldehyde) and obtain energy, dipole moment, charge on various atoms and important geometrical parameters such as bond length, bond angle, etc.

12. Perform geometry optimizations (energy minimizations) to calculate the energy of various conformations of molecules (e. g. butane, and predict the most stable conformation.

13. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane  $\sigma$  bonds and ethene, ethyne, benzene and pyridine  $\pi$  bonds.

14. Evaluation of band structure of simple solid state materials and identifying the Fermi level using any quantum chemistry software (like quantum espresso) and analyzing the results.

\*\* Other experiments may be introduced from time to time.

Textbooks:

1. Molecular Quantum Mechanics, Atkins and Friedman, 5<sup>th</sup> Edition, Oxford University Press
2. Quantum Chemistry, McQuarrie, Viva Student Edition, Viva Press

Reference Books:

1. Introductory Quantum Chemistry, AK Chandra, McGraw Hill Education (2017)
2. Introduction to Quantum Mechanics, DJ Griffiths and DF Schroeter, 3<sup>rd</sup> Edition, Cambridge University Press (2018)
3. Modern Quantum Chemistry, A Szabo and NS Ostlund, Dover Publications (1996)

4. How to use Excel in Analytical Chemistry and General Scientific data Analysis, R Levie, Cambridge University Press
5. Molecular Modelling Principles and Applications, A R Leach, Longman Publishers
6. <https://github.com/weisscharlej/SciCompforChemists>.

## Semester-IV: Magnetic Resonance Spectroscopy and Analytical Techniques (3L-0T-1P)

### Graduate Attributes

i. **Course Objective:**

Students are expected to learn about the different spectroscopic, chromatographic, electroanalytical, diffraction techniques and their applications. Relevant laboratory experiments are included to familiarize students to analytical instruments and data analysis.

ii. **Learning outcome::**

Students shall learn about spectroscopy and how chemical compounds are identified and separated using contemporary methods and instruments.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Dr. Tridib Kumar Goswami, Gauhati University, tridib@gauhati.ac.in

2) Dr. Nilamoni Nath, Gauhati University, nnath@gauhati.ac.in

3) Dr. Himangshu Prabal Goswami, Gauhati University, hpg@gauhati.ac.in

**Semester-IV: Magnetic Resonance Spectroscopy and Analytical Techniques (3L-0T-1P)**

| <b>Unit</b>                          | <b>Content</b>  | <b>Contact Hrs</b> |
|--------------------------------------|---|--------------------|
| Unit I: NMR spectroscopy             | Nuclear spin quantum number, effect of magnetic field on the nuclear spin, Zeeman effect and nuclear magneton, and Larmor precession. Radiowaves and principles of NMR spectroscopy. Chemical shift and factors affecting it. Factors affecting intensity and spectral width. NMR peak area integration relative peak positions of organic functional groups eg. alkyl halides, olefins, alkynes, aldehyde, substituted benzenes (toluene, anisole, nitrobenzenes, halobenzene, chloronitrobenzene), first order coupling (splitting of the signals: ordinary ethanol, bromoethane, dibromoethanes), Spin-spin coupling and high resolution spectra, interpretation of PMR spectra of simple organic molecules such as methanol, ethanol, acetaldehyde, acetic acid and aromatic protons. | 12                 |
| Unit II: ESR spectroscopy            | Electron spin resonance and hyperfine splitting. g value and hyperfine constant, Bohr magneton, electron Zeeman splitting, electron nuclear hyperfine splitting, illustration using simple examples like H atom, methyl radical etc.  | 5                  |
| Unit III: Mass spectrometry          | Ionization techniques (electron impact, chemical ionization), making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), separation of ions on basis of mass to charge ratio, interpretation of the mass spectrum, base peak and molecular ion peak. Fragmentation patterns of common organic molecules along with McLafferty rearrangement. Determination of empirical chemical formula from molecular ion peak and isotopic distribution.   | 8                  |
| Unit IV: Separation techniques       | Introduction to chromatography and its techniques, TLC, column chromatography, GC and HPLC.   | 5                  |
| Unit V: Electroanalytical techniques | Conductance measurements; EMF and cell reactions. Conductivity, equivalent, molar conductivity and their variation with dilution for weak and strong electrolytes. Conductometric titrations (only acid-base and acid base mixtures). Types of electrodes, standard electrode potential, cell reactions and salt bridges glass electrodes and others, concentration cells with transference and without transference, liquid junction potential and salt bridge, pH determination using hydrogen electrode and quinhydrone electrode, potentiometric titrations-qualitative treatment (acid- base, acid mixture and base and oxidation-reduction only). Zeta potential.   | 10                 |
| Unit VI: Diffraction                 | Packing of solids and how solids diffract (reflection view and scattering view) Bragg's Law, Miller indices and   | 5                  |



|                   |   |    |
|-------------------|---|----|
|                   | reciprocal lattices. Laws of crystallography. Basics of X-ray diffraction (powder and single crystal).  |    |
| Laboratory Course | <ol style="list-style-type: none"> <li>1. Determination of cell constant of a conductivity cell.</li> <li>2. Determine the equivalent conductance of a strong electrolyte (e.g. NaCl) at various concentrations and verify the Onsager equation.</li> <li>3. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.</li> <li>4. Perform the following conductometric titrations:               <ol style="list-style-type: none"> <li>(a) Strong acid vs. strong base</li> <li>(b) Weak acid vs. strong base</li> <li>(c) Mixture of strong acid and weak acid vs. strong base</li> <li>(d) Strong acid vs. weak base</li> </ol> </li> <li>4. Perform the following potentiometric titrations:               <ol style="list-style-type: none"> <li>(a) Strong acid vs. strong base</li> <li>(b) Weak acid vs. strong base</li> <li>(c) Dibasic acid vs. strong base</li> <li>(d) Potassium dichromate vs. Mohr's salt</li> </ol> </li> <li>5. Determination of basicity/proticity of a polyprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step</li> <li>6. Structure elucidation from simple proton NMR spectrum, MS.</li> <li>7. Separation of organic compounds using TLC, column chromatography.</li> </ol> | 30 |
| Recommended books | <ol style="list-style-type: none"> <li>1. Organic Spectroscopy, 3<sup>rd</sup> Edition, William Kemp.</li> <li>2. NMR Spectroscopy, 2<sup>nd</sup> Edition, Harald Günther</li> <li>3. Physical Methods in Inorganic Chemistry, Russel S. Drago.</li> <li>4. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampman, G. S. Kriz, 4<sup>th</sup> Edition.</li> <li>5. Electroanalytical methods, Bard and Faulkner.</li> <li>6. Atkins Physical Chemistry, Atkins, de Paula and Keeler, 11<sup>th</sup> Edition.</li> <li>7. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, Pearson, 2012.</li> <li>8. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press.</li> <li>9. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3<sup>rd</sup> Edition Longman, 1978.</li> </ol>   |    |

## Semester –V: Inorganic Chemistry II (3L-0T-1P)

### Graduate Attributes

i. **Course Objective:**

This course focuses on further extending the concepts of coordination chemistry along with the chemistry of main group elements, noble gases and introduction to organometallics. Intermediate level quantitative analysis of metal ions is included to give a hands-on experience to the students.

ii. **Learning outcome:**

Students shall learn about electronic and magnetic properties of coordination complexes. They shall understand the preparation, structure and properties compounds of main group elements and noble gases. Students will also learn about organometallic compounds, comprehend their bonding, stability and reactivity. The laboratory experiments shall enable the learners to separate and estimate individual ions in multicomponent systems.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Dr. Apurba Kalita, B Barooah College, apurbakalitabbc@gmail.com

2) Dr. Sanchay Jyoti Bora, Pandu College, sanchay.bora@gmail.com

3) Dr. Sonit Kumar Gogoi, Gauhati University, skgogoi@gauhati.ac.in

**Semester –V: Inorganic Chemistry II (3L-0T-1P)**

| Unit                                 | Content  | Contact Hrs |
|--------------------------------------|--|-------------|
| Unit I:<br>Coordination Chemistry IV | Electronic spectra and magnetism of coordination compounds: microstates, free ion term symbols and their splitting in tetrahedral and octahedral fields, Racah parameters, selection rules and relaxation mechanisms (vibronic coupling and spin orbit coupling), Orgel diagrams and prediction of spectral transitions, Jahn-Teller effect on electronic spectra, charge-transfer spectra, calculation of spin only and orbital contribution to magnetic moments. Spin crossover.   | 12          |
| Unit II:<br>Main Group elements      | <p>Relative stability of different oxidation states, inert pair effect, diagonal relationship, and anomalous behaviour of main group elements.</p> <p>a) Preparation and properties of ortho and para hydrogen.</p> <p>b) Preparation, structure and properties of borane (bonding in diborane, brief idea of styx number, Wade's rule), boric acid, borax, borazine, phosphazine, S<sub>4</sub>N<sub>4</sub>.</p> <p>c) Preparation and properties of oxides, superoxides, peroxides, hydrides, hydroxides, halides and carbonates of alkali and alkaline earth metals. Reactions of alkali and alkaline earth metals with liquid ammonia.</p> <p>d) Allotropes of carbon, phosphorus, and sulphur.</p> <p>e) Oxides and oxoacids of nitrogen, phosphorus, sulphur, and chlorine.</p> <p>f) Interhalogen compounds, polyhalides, pseudo halogen</p> <p>g) Hydrates, clathrates and inclusion compounds.</p> <p>h) Preparation, structure and properties of silicates, aluminosilicates.</p> | 15          |
| Unit III:Noble Gases                 | Occurrence and uses, rationalisation of inertness of noble gases, clathrates; preparation and properties of XeF <sub>2</sub> , XeF <sub>4</sub> and XeF <sub>6</sub> ; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF <sub>2</sub> ). Molecular shapes of noble gas compounds (VSEPR theory).   | 6           |

|   |  |           |
|---|--|-----------|
| <p>Unit IV:<br/>Organometallics<br/>I</p>                             | <p>Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands, 18 electron rule.</p> <p>Metal carbonyls: electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series.</p> <p>General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series.</p> <p>Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni. Pi -acceptor behaviour of CO (MO diagram of CO to be discussed), synergic bonding effect and use of IR data to explain the extent of back bonding.</p> <p>Zeise's salt: preparation and structure, evidence of synergic effect and comparison of synergic effect with that in carbonyls.</p> | <p>12</p> |
| <p><b>Laboratory:</b><br/>Inorganic<br/>quantitative<br/>analysis</p> | <ol style="list-style-type: none"> <li>1. Estimation by volumetric method of any two of the following: <ol style="list-style-type: none"> <li>a. Fe(III)- By standard <math>\text{KMnO}_4</math> solution</li> <li>b. Fe(III) – By standard <math>\text{K}_2\text{Cr}_2\text{O}_7</math> solution</li> <li>c. Cu(II) – By Iodometric method.</li> </ol> </li> <li>2. Estimation of Ni(II) by gravimetric method.</li> <li>3. Separation and estimation of individual ions in two-component systems of <ol style="list-style-type: none"> <li>a. Cu and Fe</li> <li>b. Fe and Ca</li> <li>c. Ca and Mg</li> <li>d. Cu and Ni and</li> <li>e. <math>\text{Cl}^-</math> and <math>\text{SO}_4^{2-}</math>.</li> </ol> </li> </ol>   | <p>30</p> |
| <p><b>Text/ reference<br/>Books</b></p>                               | <ol style="list-style-type: none"> <li>1. Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5<sup>th</sup> edition, Pearson Education.</li> <li>2. Principles of Inorganic Chemistry, 7<sup>th</sup> edition, Puri, Sharma, Kalia, Vishal Publishing Co.</li> <li>3. Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup> edition, Bodie Douglas, Darl Mcdaniel, John Alexander, Wiley.</li> <li>4. Advanced Inorganic Chemistry, F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Murillo, Manfred Bochmann, Wiley.</li> <li>5. Vogel's Quantitative Chemical Analysis 6<sup>th</sup> edition, J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivsankar, Pearson.</li> </ol>   |           |

## Semester-V: Organic Chemistry II (3 L- 0 T- 1 P)

### Graduate Attributes

i. **Course Objective:**

This course aims at introducing students to stereo-chemical aspects of organic reactions and their mechanisms. Students will also learn the chemical aspects of carbohydrates and terpenoids.

Familiarize the students with qualitative analysis of carbohydrates and small organic compounds with functional groups. Further, to teach students methods for identifying functional groups using IR spectroscopy.

ii. **Learning outcome:**

Students will be able to predict and recognize reactivity of organic molecules by their functional groups, and utilize this understanding for the construction of complex molecules.

Learners will be able to qualitatively analyse organic molecules and identify the functional groups by interpreting the IR spectra.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Prof. Rupam Jyoti Sarma, Gauhati University, rjs@gauhati.ac.in

2) Dr. Diganta Choudhury, B Barooah College, digantachoudhury2008@gmail.com

**Semester-V: Organic Chemistry II (3 L- 0 T- 1 P)**

| <b>Unit</b>   | <b>Content</b>   | <b>Contact Hours</b> |
|---|--|----------------------|
| Unit I:<br>Formation of carbon-carbon and carbon-heteroatom bonds | Wurtz Reaction, Wurtz-Fittig reaction, Simmons-Smith reaction; Free radical substitutions; Saytzeff and Hofmann eliminations; reagents of phosphorus, sulfur and boranes; stereospecific and stereoselective reactions; stereoselective reactions of alkenes: epoxidation reaction using mCPBA.  | 10                   |
| Unit II:<br>Reactions of active methylene compounds               | Active methylene compounds (keto-enol tautomerism): preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.   | 8                    |
| Unit III:<br>Reactions of enolates and enamines                   | Formation and stability of enolates and enamines; alkylation of enolates and enamines; aldol reaction: aldol and benzoin condensation; Claisen reaction, Claisen-Schmidt reaction, Knoevenagel condensation, Perkin reaction; Cannizzaro reaction, Wittig reaction, Favorskii reaction, Beckmann rearrangement, Benzil-Benzilic acid rearrangement; addition reactions of unsaturated carbonyl compounds; Michael addition, Wolff rearrangement.                                   | 8                    |
| Unit IV:<br>Nucleophilic reactions on the C=O groups              | Nucleophilic attack at the carbonyl group (geometrical aspects); concept of prochirality; stereoselective additions to carbonyl groups: Cram's rule, Felkin-Anh model.   | 4                    |
| Unit V:<br>Carbohydrate chemistry                                 | Classification of monosaccharides; absolute configuration of glucose and fructose, epimers and anomers; mutarotation; determination of ring size of glucose and fructose; conformations of glucose (Fischer, Haworth and stereoscopic projections); interconversions of aldoses and ketoses; Killiani Fischer synthesis and Ruff degradation; disaccharides: structure elucidation of maltose, lactose and sucrose. Polysaccharides -structures of starch, cellulose and glycogen. | 9                    |
| Unit VI:<br>Terpenes  | Occurrence of terpenes; structure and classification of terpenes, isoprene rule; synthesis of citral, neral and $\alpha$ -terpineol; biosynthesis of limonene, pinene, carvone ( <i>via</i> isopentenyl pyrophosphate).  | 6                    |

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| Lab Course        | <p>1. Qualitative analysis of carbohydrates: aldoses and ketoses, reducing and non-reducing sugars.</p> <p>2. (a) Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, phenols, amines, nitro, carboxylic acids and carbonyl compounds).</p> <p>(b) Interpretation of infrared (IR) spectra of simple organic compounds.</p> <p><i>The student is required to learn about identification of functional groups of simple organic compounds by interpreting the IR spectra. The spectra may be recorded and/or provided to the students from literature.</i></p>   | 30 |
| Recommended books | <ol style="list-style-type: none"> <li>1. Organic Chemistry, Jonathan Clayden, Nick Greeves, Stuart Warren, 2<sup>nd</sup> Edition.</li> <li>2. Principles of Organic Synthesis, R. O. C. Norman, J. M. Coxon, 3<sup>rd</sup> Edition.</li> <li>3. Advanced Organic Chemistry, R. Bruckner.</li> <li>4. Organic Chemistry, G. M. Loudon, 4<sup>th</sup> Edition.</li> <li>5. Organic Chemistry, R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee, 7<sup>th</sup> Edition.</li> <li>6. Organic Chemistry, Volume 2, I. L. Finar, 5<sup>th</sup> Edition.</li> <li>7. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, Pearson, 2012.</li> <li>8. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press.</li> <li>9. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3<sup>rd</sup> Edition Longman, 1978.</li> </ol> |    |

## Semester-V: Reaction Dynamics (3L-0T-1P)

### Graduate Attributes

i. ***Course Objective:***

The aim of this course is to teach students reaction dynamics with emphasis on order and molecularity of reactions, rate laws and rate equations, equilibrium and steady states, collision theory etc.

ii. ***Learning outcome***

Students shall learn how to mathematically model chemical reactions and evaluate the necessary rates of chemical reactions. They shall also be able to comprehend enzyme action in human physiology. Students shall be able to visualize complex reaction mechanisms via mathematical modeling and develop an analytical thinking ability.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer (Name, Institution, email id):**

1) Dr. Dhriti Mahanta, Gauhati University, mdhriti@gauhati.ac.in

2) Dr. Dhruva Jyoti Kalita, Gauhati University, dhrubajyoti.kalita@gauhati.ac.in



**Semester V – Reaction Dynamics (3L-0T-1P)**

| Unit                           | Content  | Contact Hrs |
|--------------------------------|--|-------------|
| Unit I:<br>Kinetics I          | Order and molecularity of reactions. Rate laws and rate equations for zero, first and second order reactions ( $2A \rightarrow P$ , $A+B \rightarrow P$ ): their derivations, graphical representations and examples. Expressing the rate laws in terms of volume and pressure of reactants. Experimental determination of order of reactions (half-life method and initial rate method). Temperature dependence of reaction rate, energy of activation (its connection to Gibbs free energy). Arrhenius equation, energy of activation. Pre-exponential Factor and failure of Arrhenius Equation.   | 9           |
| Unit II:<br>Kinetics II        | Difference between equilibrium and steady state. Limiting reagents, rate-determining step and steady-state approximation – explanation with suitable examples (eg. dissociation of HBr and acetaldehyde). Opposing reactions, consecutive reactions and parallel reactions (with examples and explanation of kinetic and thermodynamic control of products; all steps first order). Idea on explosive reactions. Enzyme catalysis: Derivation of Michaelis-Menten equation and interpretation of Lineweaver-Burk Plots. Eadie- Hofstee plot. Turn-over number. Oscillating reactions.  | 14          |
| Unit III:<br>Reaction Dynamics | Collision theory (detailed treatment). Modeling the Preexponential factor. Sphere of influence and collision cross section, Equivalence between Arrhenius and Collision theory. Failure of Collision theory. Physical interpretation of reaction co-ordinates and potential energy surfaces. Activated complex theory (detailed treatment). Thermodynamic formulation and derivation of Eyring equation. Evaluation of Arrhenius pre-exponential factor from transition state theory. Common examples where transition states have been experimentally identified or predicted.<br>Chemically and Diffusion controlled reactions with examples. Primary and secondary salt effects with examples.<br>Derivation of Bronsted-Bjerrum Equation and its graphical representation. Lindemann and Hinshelwood theory of unimolecular reaction and graphical representation. | 22          |

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| Laboratory experiments   | <ol style="list-style-type: none"> <li>1. Determine the rate constant of the acid catalyzed hydrolysis of methyl acetate.</li> <li>2. Determine the rate constant of saponification of ethyl acetate.</li> <li>3. Determine the activation energy of the hydrolysis of methyl acetate catalyzed by hydrochloric acid.</li> <li>4. Verify the Freundlich isotherm for the adsorption of oxalic acid on activated charcoal.</li> <li>5. Verify the Langmuir isotherm for the adsorption of acetic acid on activated charcoal.</li> </ol> <p>Determine the critical micelle concentration of a surface-active agent by surface tension measurements.</p> <ol style="list-style-type: none"> <li>6. Study the kinetics of the Iodide-persulphate reaction by Initial rate method.</li> <li>7. Theory and computer aided linear curve-fitting techniques (eg. first order kinetics using least squares) and evaluation of errors and standard deviations.</li> </ol> | 30 |
| <p>Text Books:</p> <ol style="list-style-type: none"> <li>1. Atkins' Physical Chemistry, Atkins, de Paula and Keeler</li> <li>2. Chemical Kinetics and Reaction Dynamics, Paul L. Houston</li> </ol> <p>Reference books:</p> <ol style="list-style-type: none"> <li>1. A Textbook of Physical Chemistry, K. L. Kapoor, Volume V, Macmillan</li> <li>2. Principles of Physical Chemistry, Puri, Sharma, Pathania, 48<sup>th</sup> edition, Vishal Publication.</li> <li>3. Physical Chemistry: P C Rakshit</li> <li>4. Physical Chemistry: A Molecular Approach by McQuarrie and Simon</li> <li>5. Chemical Kinetics by Kaith J Laidler, McGraw-Hill</li> </ol> |   |    |

## Semester-V: Light-Matter Interaction (3L-0T-1P)

### Graduate Attributes

i. **Course Objective:**

This paper is focused on fundamental theory and application of photochemistry and various spectroscopic techniques such as rotational, vibrational, electronic and Raman spectroscopy. The accompanying laboratory course aims to introduce the students to various computational/experimental tools.

ii. **Learning outcome:**

Students shall learn about the theory of photochemistry, spectroscopy and their application in chemistry. They shall use the knowledge gained from the quantum theories to identify unknown chemical compounds using modern techniques. The experiments performed in the laboratory course shall enable the learners to analyze/estimate various analytes using different techniques.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Dr. Himangshu Prabal Goswami, Gauhati University, hpg@gauhati.ac.in

2) Dr. Dhriti Mahanta, Gauhati University, mdhriti@gauhati.ac.in

**Semester V – Light-Matter Interaction (3L-0T-1P)**

| <b>Unit</b>                | <b>Content</b>  | <b>Contact Hrs</b> |
|----------------------------|---|--------------------|
| Unit I:<br>Photochemistry: | Laws of photochemistry: Grotthus-Draper law, Stark-Einstein law of photochemical equivalence. Beer-Lambert law (for solids and liquids) and limitations. Quantum yield and its measurement for photochemical processes. Actinometry. Photostationary state. Photosensitized reactions (with examples). Jablonski diagrams: internal conversion, intersystem crossing, fluorescence and phosphorescence. Frank Condon principle. Primary and secondary processes in photochemical reactions.   | 10                 |
| Unit II:<br>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. Absorption cross section and Einstein's coefficients. Difference between atomic and molecular spectra. Born- Oppenheimer approximation. Separation of molecular energies into translational, rotational, vibrational and electronic degrees of freedom. Factors affecting intensities and width of spectral lines. Microwave (pure rotational) spectra of diatomic molecules. Selection rules and transition dipole moment. Structural information derived from rotational spectroscopy. IR Spectroscopy: Selection rules, IR spectra of diatomic molecules and organic compounds having functional groups. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies. Effect of hydrogen bonding (inter and intramolecular) and substitution on vibrational frequencies. Electronic Spectroscopy: electronic excited states and selection rules. Free electron model and its application to electronic spectra of polyenes. Vibronic and spin orbit coupling. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts. Woodward-Fieser rules. Qualitative treatment of Raman effect. Elements of rotational Raman spectra Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference. Rule of mutual exclusion. | 35                 |

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| <p>Laboratory (minimum of seven to be performed)</p> | <ol style="list-style-type: none"> <li>1. Calculation of the rotational constant for simple diatomic systems (eg. N<sub>2</sub>, F<sub>2</sub>, O<sub>2</sub>) via quantum chemistry softwares.</li> <li>2. Calculation of the optimum bond length by hand (theoretical) from the rotational constant via the rigid rotor approximation for a diatomic molecule.</li> <li>3. To perform a series of single point calculations above and below equilibrium bond distance to generate a potential energy surface (PES) followed by a frequency calculation on the optimized geometry. Use of the resulting fundamental frequency to calculate the force constant of the bond.</li> <li>4. Simulating the IR spectra of simple nonlinear molecules (eg. water, ammonia, boron trifluoride etc) using quantum chemistry software and assign the spectra to the corresponding vibrational modes.</li> <li>5. To study the 200-500 nm absorbance spectra of KMnO<sub>4</sub> and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> (in dil. H<sub>2</sub>SO<sub>4</sub>) and determine the <math>\lambda_{\max}</math> values. Calculate the energies of the two transitions in different units (J molecule<sup>-1</sup>, kJ mol<sup>-1</sup>, cm<sup>-1</sup>, eV).</li> <li>6. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>.</li> <li>7. Record the 200-350 nm UV spectra of organic compounds ( eg. acetone, acetaldehyde, 2-propanol, acetic acid) and interpret the spectra. Compare these experimental results with associated theoretical rules.</li> <li>8. Complete spectral analysis of the given (or recorded) vibration-rotation spectrum of HCl (g).</li> <li>9. Verify Lambert-Beer's law and determine the concentration of CuSO<sub>4</sub>/KMnO<sub>4</sub>/K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> in a solution of unknown concentration</li> <li>10. Determine the concentrations of KMnO<sub>4</sub> and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> in a mixture.</li> <li>11. Study the kinetics of iodination of propanone in acidic medium.</li> <li>12. Determine the amount of iron present in a sample using 1,10-phenanthroline.</li> <li>13. Determine the dissociation constant of an indicator (phenolphthalein).</li> <li>14. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.</li> </ol> | <p>30</p> |
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Text Books:

1. Fundamentals of Molecular Spectroscopy, C N Banwell, 4<sup>th</sup> Edition, McGraw-Hill
2. Atkins Physical Chemistry, P Atkins, J Paula and J Keeler, 11<sup>th</sup> Edition, Oxford University Press. 2018

Reference Books:

1. Introduction to Spectroscopy, DL Pavia, GL Lampman, GS Kriz and J R Vyvyan, 5<sup>th</sup> Edition, Cengage India Private Limited, 2015
2. Introduction to Molecular Spectroscopy: GM Barrow, McGraw Hill, 1992.
3. Basic Atomic and Molecular Spectroscopy, Vol 11, J M Hollas, Royal Society of Chemistry, 2002.
4. Symmetry and Spectroscopy: an introduction to vibrational and electronic spectroscopy, DC Harris and M D Bertolucci, 1989, Dover Publications
5. Molecular Spectroscopy, JL McHale, 2<sup>nd</sup> Edition, CRC Press
6. Atomic and Molecular Spectroscopy: Basic Concepts and Applications. Rita Kakkar, 2<sup>nd</sup> Edition, S Chand Publishing

## Semester-VI: Inorganic Chemistry III (3L-0T-1P)

### Graduate Attributes

i. **Course Objective:**

This course aims at giving students the introduction to inorganic reaction mechanisms and bioinorganic chemistry. Moreover, this course emphasizes on organometallic chemistry with reference to transition metal- $\pi$  bound complexes, metal-carbenes and organometallic catalysis. The laboratory course intends to introduce students to preparation and characterization of coordination complexes and double salts.

ii. **Learning outcome:**

Students shall understand the mechanisms of inorganic reactions and the role of metal ions in biological processes and therapeutic activities. They will be acquainted with the synthesis, structure and reactivity of various organometallic compounds, and their application in organometallic catalysis. Furthermore, the students will understand the importance of organometallic catalysis in the synthesis of industrially important compounds. The laboratory experiments will enable the learners to synthesize metal complexes and double salts and their characterization by various analytical techniques.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Dr. Sanfaori Brahma, Gauhati University, sanfaori@gauhati.ac.in

2) Dr. Apurba Kalita, B Barooah College, apurbakalitabc@gmail.com

## Semester VI- Inorganic Chemistry III (3L-0T-1P)

| Unit                               | Content  | Contact Hrs |
|------------------------------------|--|-------------|
| Unit I<br>Coordination Chemistry-V | <p>Introduction to inorganic reaction mechanisms. Stepwise and overall formation constants, the chelate effect, thermodynamic and kinetic stability of complexes, chelate effect and its applications in analytical chemistry and biology.</p> <p>Substitution reactions in octahedral complexes, factors affecting the substitution reaction, effect of acid and bases on substitution reaction of octahedral complexes.</p> <p>Substitution reaction of square planar complexes, trans-effect, theories of trans effect, trans effect in synthesis of square planar complexes.</p> <p>Electron transfer reactions (elementary ideas only)</p>  | 15          |
| Unit II<br>Organometallics II      | <p>Metal alkenes, alkynes and allyls: synthesis, structure, bonding and reactivity.</p> <p>Metal carbene: synthesis, structure, bonding and reactivity</p> <p>Ferrocene: preparation and reactions (acetylation, alkylation, metallation, Mannich condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene</p> <p>Fundamentals of organometallic reactions: oxidative addition, reductive elimination, insertion and <math>\beta</math>-hydride elimination reaction.</p> <p>Transition metals in catalysis.</p> <p>Study of the industrial processes and their mechanism: alkene hydrogenation (Wilkinson's Catalyst), hydroformylation (Co catalysts), Wacker Process, synthetic gasoline (Fischer Tropsch reaction), Monsanto acetic acid process.</p> | 15          |
| Unit III<br>Bioinorganic Chemistry | <p>Essential and trace metals in biology. Effect of deficiency of essential metal ions. Toxic effect of metal ions (Fe, Cu, Hg, Pb, Cd and As), chelate therapy, cisplatin as anticancer drug.</p> <p>Storage and transport of iron, active transport of ions (sodium -potassium pump)</p> <p>Active site structure and function of haemoglobin (cooperativity and Bohr effect), myoglobin, hemocyanin, hemerythrin, rubredoxin, ferredoxin (<math>\text{Fe}_2\text{S}_2</math>, <math>\text{Fe}_4\text{S}_4</math>), cytochrome P450, superoxide dismutase, carbonic anhydrase and carboxypeptidase, nitrogenase enzyme, vitamin B<sub>12</sub></p>   | 15          |



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| <p><b>Laboratory:</b><br/>Inorganic<br/>Preparation</p> | <p>Following compounds should be prepared and tested for the presence of ions qualitatively. IR and UV-Visible spectra of these complexes should be recorded, interpreted and discussed.</p> <ul style="list-style-type: none"> <li>i) Preparation of Mohr's Salt, chrome alum and potash alum</li> <li>ii) Cis and trans <math>K[Cr(C_2O_4)_2 \cdot (H_2O)_2]</math><br/>Potassium dioxalatodiaquachromate (III)</li> <li>iii) Potassium tris(oxalato)ferrate(III)</li> <li>iv) Vanadyl bis(acetylacetonate)</li> <li>v) Cu-thiourea complex</li> <li>vi) Acetylation of ferrocene and purification of mono and bis derivatives by column chromatography.</li> </ul> | <p>30</p> |
| <p>Text/ Reference<br/>Books</p>                        | <ol style="list-style-type: none"> <li>1. Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5<sup>th</sup> edition, Pearson Education.</li> <li>2. Principles of Inorganic Chemistry, 7<sup>th</sup> edition, Puri, Sharma, Kalia, Vishal Publishing Co.</li> <li>3. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, University Science Books.</li> <li>4. The Organometallic Chemistry of the transition Metals, Robert H. Crabtree, 4<sup>th</sup> edition, Wiley</li> <li>5. Inorganic syntheses, series, Wiley.</li> </ol>   |           |

## Semester-VI: Organic Chemistry III (3 L- 0 T- 1 P)

### Graduate Attributes

i. **Course Objective:**

This course aims at introducing the students to photo-chemical and pericyclic organic reactions. The learners shall be able to understand the chemistry of polynuclear aromatic hydrocarbons, organometallic compounds and their reactions.

Experiments are aimed at introducing the students to natural product extraction, photochemical organic transformations and estimation of organic compounds.

ii. **Learning outcome:**

Students will be able to recognize and explain the mechanisms of photochemical and pericyclic reactions and apply mechanistic concepts to predict the outcome of synthetic reactions. Students will be introduced to the preparation, structure and reactivity of polyaromatic hydrocarbons and organometallic compounds.

Students will develop the skill set to extract important organic components from natural samples, estimate organic compounds and perform photochemical conversion.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Prof. Rupam Jyoti Sarma, Gauhati University, rjs@gauhati.ac.in

2) Dr. Ranjit Thakuria, Gauhati University, ranjit.thakuria@gauhati.ac.in

**Semester-VI: Organic Chemistry III (3 L- 0 T- 1 P)**

| <b>Unit</b>                        | <b>Content</b>  | <b>Contact Hours</b> |
|------------------------------------|---|----------------------|
| Unit I: Photochemistry             | Electron excitation in organic molecules (alkenes and carbonyl compounds); fate of electronically excited molecules; singlet and triplet states; photoreduction of carbonyl compounds; photoaddition of alkenes to carbonyl compounds (Paterno-Buchi reaction); photoaddition of alkenes to aromatic compounds; photorearrangement (cis-trans isomerization, intramolecular cyclization of dienes); photochemical fragmentation (photolysis of carbonyl compounds: Norrish type I and type II reactions).   | 10                   |
| Unit II: Pericyclic reactions      | Cycloadditions: general description of the Diels-Alder reaction; frontier orbital description of [4+2] cycloadditions; regioselectivity in Diels-Alder reactions; Woodward-Hoffmann description of the Diels-Alder reaction; photochemical [2+2] cycloadditions; thermal [2+2] cycloadditions.<br>Sigmatropic reactions: conditions for sigmatropic reactions, orbital descriptions of [3,3]-sigmatropic rearrangements; Cope rearrangement<br>Electrocyclic reactions: conditions for [4 $\pi$ +2] and [4 $\pi$ ] electrocyclic reactions; conrotatory and disrotatory reactions.  | 15                   |
| Unit III: Polynuclear hydrocarbons | Preparation, structure and reactions of naphthalene, phenanthrene and anthracene.   | 5                    |
| Unit IV: Organometallic chemistry  | General introduction to preparation, structure and reactivity of organolithium, organomagnesium (Schlenk equilibrium), organocopper, organozinc, organoaluminum, and organoboron reagents; general methods of preparation: deprotonation, metal-halogen exchange, transmetallation; directed metallation.   | 15                   |
| Laboratory Course                  | 1. Extraction of D-limonene from orange peel by the conventional method/ using liquid CO <sub>2</sub> prepared from dry ice.<br>2. Extraction of caffeine from commercially available tea leaves.<br>3. Photoreduction of benzophenone to benzopinacol in the presence of sunlight/UV irradiation.<br>4. Organic estimations (any three):<br>(i) Estimation of glycine by Sorenson's formalin method.<br>(ii) Study of the titration curve of glycine (by pH metric methods).<br>(iii) Determination of Iodine number of vegetable oil or a fat.<br>(iv) Saponification value of vegetable oil or a fat.<br>(v) Estimation of glucose by titrimetric methods. | 30                   |

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| <p>Recommended books</p> | <ol style="list-style-type: none"> <li>1. Foundations of Photochemistry, K. K. Rohatgi-Mukherjee, 3<sup>rd</sup> Edition.</li> <li>2. Principles of Organic Synthesis, R. O. C. Norman, J. M. Coxon, 3<sup>rd</sup> Edition.</li> <li>3. Mechanism and Theory in Organic Chemistry, T. H. Lowry, K. S. Richardson.</li> <li>4. Pericyclic Reactions, Vinod Kumar, S. P. Singh.</li> <li>5. Organic Chemistry, Volume 1, I. L. Finar, 5<sup>th</sup> Edition.</li> <li>6. Organic Chemistry, Jonathan Clayden, Nick Greeves, Stuart Warren, 2<sup>nd</sup> Edition.</li> <li>7. Modern Methods of Organic Synthesis, W. Carruthers, I. Coldham, 4<sup>th</sup> Edition.</li> <li>8. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, Pearson, 2012.</li> <li>9. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press.</li> <li>10. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3<sup>rd</sup> Edition Longman, 1978.</li> </ol> |
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## Semester-VI: Equilibria and Electrochemistry (3L-0T-1P)

### Graduate Attributes

i. **Course Objective:**

The aim of this course is to introduce students to primarily two areas of physical chemistry- equilibria and electrochemistry. Discussion of equilibria encompasses- chemical, ionic and phase equilibria. The learners are expected to learn various laws of electrochemistry, measurements of conductance, applications of electrolysis in industry, electrochemical cells etc. The accompanying laboratory course is designed to introduce students to various experiments using pHmetry, conductometry, calorimetry etc.

ii. **Learning outcome:**

Students shall understand how dynamic equilibrium works in chemical reactions. They shall be introduced to ionics, phases and electrochemical systems.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Dr. Debajyoti Mahanta, Gauhati University, debam@gauhati.ac.in

2) Dr. Sanjib Deuri, M C College, Barpeta, s\_deuri@yahoo.com

### Semester VI – Equilibria and Electrochemistry (3L-0T-1P)

| Unit                        | Content  | Contact Hrs |
|-----------------------------|--|-------------|
| Unit I: Chemical Equilibria | Equilibrium of homogeneous and heterogeneous systems. Law of mass action, derivation of expression of equilibrium constants; temperature, pressure and concentration dependence of equilibrium constants ( $K_P$ , $K_C$ , $K_X$ ), their applications. Le Chatelier's principle of dynamic equilibrium and its applications.  | 5           |
| Unit II: Ionic Equilibria   | Introduction to ionic equilibrium. Ionic product. Common ion effect: its application. Acid-base equilibria. Dissociation constants of mono and dibasic acids. pH scale, pH of very dilute and very concentrated solutions. Concept of strengths of solutions (molarity, normality and molality, difference between mass of a substance and amount of a substance). Calculation of strengths of acid and basic mixtures. pH titration curves of acid mixtures, salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions and derivation of Henderson-Hasselbalch equation (for mono and dibasic acids). Solubility and solubility product of sparingly soluble salts – applications of solubility product principle with special reference to inorganic group separation. Explanation of inorganic group separation table using Le Chatelier's principle, solubility product and common ion effect. | 10          |
| Unit III: Phase Equilibria  | Definitions of phase, component and degrees of freedom. Gibb's phase rule and its derivations. Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems, with applications. Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions. Fractional distillation of binary miscible liquids (ideal and nonideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation. Nernst distribution law. Solvent extraction.  | 15          |
| Unit IV: Electrochemistry   | Conductivity, equivalent and molar conductivity and their properties; Kohlrausch law; Debye-Huckel Theory, Debye-Huckel Limiting Law, Debye Hückel Onsager equation (no derivation required); Ionic velocities, mobilities, transference numbers and its experimental determination using Hittorf and moving boundary methods; Applications of conductance measurement; Quantitative aspects of Faraday's laws of electrolysis, applications of electrolysis in metallurgy and industry; Electrolytic and galvanic cells, Electromotive force of a cell, Nernst equation; Standard   | 15          |

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|  | <p>electrode potential, Electrochemical series; Concentration cells with and without transference; Applications of EMF measurements including potentiometric titrations.</p> <p>Electrochemistry behind standard Pb Batteries and rechargeable Li-ion batteries.</p>  |           |
| <p>Laboratory experiments (a minimum of seven experiments to be performed)</p>   | <ol style="list-style-type: none"> <li>1. pH metric titration of strong acid vs. strong base,</li> <li>2. pH metric titration of weak acid vs. strong base.</li> <li>3. Determination of dissociation constant of a weak acid.</li> <li>4. Determination of critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.</li> <li>5. Determine the transition temperature of a salt hydrate.</li> <li>6. Construction of phase diagram (freezing point curve) using ignition tube method for two- component simple eutectic system.</li> <li>7. Construction of phase diagram (freezing point curve) using ignition tube method for two- component congruently melting compound forming system.</li> <li>8. Study the distribution of iodine between water and kerosene/carbon tetrachloride.</li> <li>9. Determine the association factor of benzoic acid in benzene by distribution of benzoic acid between water and benzene.</li> <li>10. Determine the vapour pressure of water at different temperatures and hence evaluate the enthalpy of vaporization of water.</li> <li>11. Determine the partition coefficient of ammonia between water and chloroform and also determine the formula of copper-ammonia complex.</li> <li>12. Study of the solubility of benzoic acid in water and determination of <math>\Delta H</math>.</li> </ol> <p>** Other experiments may also be introduced.</p> | <b>30</b> |
| <p>Textbooks:</p> <ol style="list-style-type: none"> <li>1. Atkins Physical Chemistry, P Atkins, J de Paula and J Keeler, 11<sup>th</sup> Edition, Oxford University Press.</li> <li>2. Principles of Physical Chemistry, Puri, Sharma, Pathania, 48<sup>th</sup> Edition, Vishal Publishing Com.</li> </ol> <p>Reference Books:</p> <ol style="list-style-type: none"> <li>1. Physical Chemistry: RS Berry, SA Rice and J Ross, 2<sup>nd</sup> Edition, Oxford University Press.</li> <li>2. Physical Chemistry, P C Rakshit, Enlarged Seventh Edition, Sarat Book House.</li> <li>3. Modern Electrochemistry, J O'M Bockris and AKN Reddy, Volume I: Ionics, Second Edition, Springer</li> </ol> |   |           |

## Semester-VI: Industrial Chemistry (3L-0T-1P)

### Graduate Attributes

i. **Course Objective:**

This course provides an introduction to the various industrial gases and inorganic chemicals, their manufacturing processes, applications, storage and the hazards of handling them. The students are also expected to learn the synthetic processes, properties and the utility of the industrially important inorganic materials.

ii. **Learning outcome:**

Students shall acquire knowledge of industrially important chemical processes. They shall know the extraction processes and the chemistry of firecrackers, ceramics, glass and cements.

No. of Required Classes: 45 (Theory) + 30 (Practical)

No. of Contact Classes: 45 (Theory) + 30 (Practical)

No. of Non-Contact Classes:

iii. **Particulars of Course Designer** (Name, Institution, email id):

1) Dr. Akhtar Hussain, Handique Girls College, akhtariisc@gmail.com

2) Dr. Sonit Kumar Gogoi, Gauhati University, skgogoi@gauhati.ac.in



**Semester VI: Industrial Chemistry (3L-0T-1P)**

| Units  | Content  | Contact Hrs |
|--|--|-------------|
| Unit I:<br>Industrial Gases and Common Inorganic Chemicals | <p><b>Industrial Gases:</b> large scale production, uses, storage and hazards in handling of the following gases: hydrogen, oxygen, nitrogen, chlorine, argon, helium, acetylene, phosgene.</p> <p><b>Inorganic Chemicals:</b> manufacture, application and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, bleaching powder, hydrogen peroxide, potash alum, and potassium permanganate.</p>   | 9           |
| Unit II:<br>Silicate Industries                            | <p><b>Glass:</b> Glassy state and its properties, classification (silicate and non-silicate glasses).<br/>Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, borosilicate glass, armoured glass, coloured glass, photosensitive glass.</p> <p><b>Ceramics:</b> important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, semiconducting oxides.</p> <p><b>Cements:</b> classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.</p> | 8           |
| Unit III:<br>Fertilizers                                   | <p>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.</p>   | 6           |
| Unit IV:<br>Surface Coatings                               | <p>Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Pigments, toners and lake pigments, fillers, thinners, enamels, emulsifying agents.</p> <p>Special paints (heat retardant, fire retardant, eco-friendly and plastic paint), dyes, wax polishing, water and oil paints, additives, metallic coatings (electrolytic and electroless), metal spraying and anodizing.</p>   | 8           |
| Unit V:<br>Alloys  | <p>Classification of alloys, ferrous and non-ferrous alloys, specific properties of elements in alloys. Manufacture composition and properties of different types of steels (stainless steel, Ni-steel, Cr-steel).<br/>Brass, bronze and Cu-Ni alloy.</p>  | 6           |

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|---|---|----|
| Unit VI:<br>Catalysis                     | Catalysts and their industrial applications, deactivation or regeneration of catalysts. Phase transfer catalysts, application of zeolites as catalysts.   | 4  |
| Unit VII:<br>Pyrotechnics and Propellants | Firecrackers- composition and effect.<br>Fire extinguishers-types and use.<br>Car airbag chemistry.<br>Introduction to rocket propellants.  | 4  |
| <b>Laboratory</b>                         | <ol style="list-style-type: none"> <li>1. Determination of free acidity in ammonium sulphate fertilizer.</li> <li>2. Estimation of calcium in calcium ammonium nitrate fertilizer.</li> <li>3. Estimation of phosphoric acid in superphosphate fertilizer.</li> <li>4. Electroless metallic coatings on ceramic and plastic material.</li> <li>5. Determination of composition of dolomite (by complexometric titration).</li> <li>6. Analysis of (Cu, Ni); (Cu, Zn) in alloy or synthetic samples.</li> <li>7. Analysis of Cement.</li> <li>8. Preparation of pigment (zinc oxide).</li> </ol> | 30 |
| Text Books and Reference Books            | <ol style="list-style-type: none"> <li>1. Industrial Chemistry, Vol-I, E. Stocchi, Ellis Horwood Ltd. UK.</li> <li>2. Industrial Chemistry-I &amp; Industrial Chemistry-II, B. K. Sharma, Krishna's Educational Publishers.</li> <li>3. Riegel's Handbook of Industrial Chemistry, J. A. Kent, CBS Publishers.</li> <li>4. R. Gopalan, D. Venkappayya, S. Nagarajan, Engineering Chemistry, Vikas Publications.</li> <li>5. Engineering Chemistry, B. K. Sharma, Goel Publishing House.</li> </ol>  |    |