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

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

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

Unit	Content	Contact Hours
Unit I: 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 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 (Δ_o, Δ_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: 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: 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. Diagrammatic representation of potential data (Latimer diagram, Frost diagram, Pourbaix diagram).	6
Unit VI: 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. Actinoids: electronic configuration, oxidation states, magnetic properties, comparison with lanthanides.	6

Unit VII: Nuclear 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
Laboratory: Inorganic Qualitative Analysis	Qualitative analysis of mixtures containing four cations and anions. Emphasis should be given to the understanding of reactions. The following radicals are suggested: CO_3^{2-} , NO_2^-, S^{2-}, SO_3^{2-}, $S_2O_3^{2-}$, CH_3COO^-, F^-, Cl^-, Br^-, I^-, NO_3^-, BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH_4^+, K^+, Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+} Mixtures should preferably contain one interfering anion, or insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) or combination of anions such as CO_3^{2-} and SO_3^{2-}, NO_2^- and NO_3^-, Cl^- and Br^-, Cl^- and I^-, Br^- and I^-, NO_3^- and Br^-, NO_3^- and I^-. Spot tests should be done whenever possible.	30
Text Books/ Reference Books	1. Inorganic Chemistry, G.L. Meissler and D. A. Tarr, 5th edition, Pearson. 2. Inorganic Chemistry, P. Atkins, Overtone Rourke, Weller and Armstrong 5th edition, Oxford. 3. Principles of Inorganic Chemistry, 7th edition, Puri, Sharma, Kalia, Vishal Publishing Co. 4. Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5th edition, Pearson Education. 5. Advanced Inorganic Chemistry, F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Murillo, Manfred Bochmann, Wiley. 6. Vogel's Qualitative Inorganic Analysis, 7th Edition, G. Svehla, B Sivasankar, Pearson.	

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)

Unit	Content	Contact Hours
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. Preparation and reactions of acid chlorides, anhydrides, esters and amides; comparison of nucleophilic sustitution 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. General methods for preparation of nitro compounds, nitriles and isonitriles and important reactions.	8
Unit III: Amino acids, peptides and proteins	α-Amino acids (synthesis and reactions); zwitterions, p*K*a 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	1. Organic preparations (any two from each): benzoylation of organic compounds: amines (aniline, toluidines, anisidine) and phenols (phenol, *β*-naphthol, salicylic acid) by the following methods: (i) Using conventional method. (ii) Using green chemical approach. 2. Organic preparations (any three): (i) Bromination of acetanilide by conventional methods. (ii) Nitration of salicylic acid using ceric ammonium (green chemistry approach). (iii) Selective reduction of *m*-dinitrobenzene to *m*-nitroaniline (iv) Oxidation of ethanol/ isopropanol (iodoform reaction). (v) Aldol condensation using either conventional or green method. (vi) Benzil-Benzilic acid rearrangement. 3. Chromatography: (a) Separation of a mixture of two amino acids by ascending paper chromatography; (b) Separation of a mixture of *o*- and *p*-nitrophenol or *o*- and *p*-nitroaniline by thin layer chromatography (TLC).	30
Recommended books	1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith 7th Edition. 2. Organic Chemistry, Jonathan Clayden, Nick Greeves, Stuart Warren, 2nd Edition. 3. Principles of Organic Synthesis, R. O. C. Norman, J. M. Coxon, 3rd Edition. 4. Organic Chemistry, P. Y. Bruice, 8th Edition. 5. Organic Chemistry, Volume 2, I. L. Finar, 5th Edition. 6. Organic Chemistry, P. Y. Bruice, 8th Edition. 7. Organic Spectroscopy, 3rd Edition, William Kemp. 8. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampman, G. S. Kriz, 4th Edition. 9. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, Pearson, 2012. 10. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press. 11. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3rd Edition Longman, 1978.	

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: Quantum Theory	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. 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. Rotational Motion and Energy: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels. 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. 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.	**37**
Unit II: 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)	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 MSExcel/LibreOffice etc or simple programming language (GWBasic, FORTRAN, python etc) 2. Plotting the wavefunction and the energy expressions for particle in a box for n =1,2 and 3 using any spreadsheet software such as MSExcel/LibreOffice etc or simple programming language (GWBasic, FORTRAN, python etc). 3. Numerical evaluation of the 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 MSExcel/LibreOffice etc or simple programming language (GWBasic, FORTRAN, python etc). 4. Plotting simple one-dimensional intermolecular potential energies (eg. harmonic, anharmonic, Lennard-Jones potential etc)	**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+ 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 σ bonds and ethene, ethyne, benzene and pyridine π 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, 5th 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, 3rd 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)

Unit	Content	Contact Hrs
Unit I: NMR spectroscopy	Nuclear spin quantum number, effect of magnetic field on the nuclear spin, Zeeman effect and nuclear magneton, and Larmor precision. 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, bromoehane, dibromoehanes), 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	1. Determination of cell constant of a conductivity cell. 2. Determine the equivalent conductance of a strong electrolyte (e.g. NaCl) at various concentrations and verify the Onsager equation. 3. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid. 4. Perform the following conductometric titrations: (a) Strong acid vs. strong base (b) Weak acid vs. strong base (c) Mixture of strong acid and weak acid vs. strong base (d) Strong acid vs. weak base 4. Perform the following potentiometric titrations: (a) Strong acid vs. strong base (b) Weak acid vs. strong base (c) Dibasic acid vs. strong base (d) Potassium dichromate vs. Mohr's salt 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 6. Structure elucidation from simple proton NMR spectrum, MS. 7. Separation of organic compounds using TLC, column chromatography.	30
Recommended books	1. Organic Spectroscopy, 3rd Edition, William Kemp. 2. NMR Spectroscopy, 2nd Edition, Harald Günther 3. Physical Methods in Inorganic Chemistry, Russel S. Drago. 4. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampman, G. S. Kriz, 4th Edition. 5. Electroanalytical methods, Bard and Faulkner. 6. Atkins Physical Chemistry, Atkins, de Paula and Keeler, 11th Edition. 7. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, Pearson, 2012. 8. V. K. Ahluwalia, S. Dhingra, Comprehensive Practical Organic Chemistry, University Press. 9. F. G. Mann, B. C. Saunders, Practical Organic Chemistry, 3rd Edition Longman, 1978.	