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):

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

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Unit	Content	Contact Hours
Unit I: 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 Ψ and Ψ^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: Periodicity and chemical behaviour	Effective nuclear charge; Slater's Rule; covalent and ionic radii, ionization energies, electronegativity (various scales), electron affinities	3
Unit III: 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: 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: 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: Electronic effects in organic molecules	Concept of electrophiles and nucleophiles; inductive effects; resonance, conjugation and delocalisation.	3

Unit VII: Gaseous 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: Liquid 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

Laboratory Course I	1. Introduction to laboratory apparatus and safety measures in laboratory, 2. Calibration of apparatus (volumetric flask, thermometer, melting point apparatus etc.) **Group A** (a) Preparation of normal and molar solution, for example KCl, $Na_2C_2O_4$, HCl, H_2SO_4 etc. (Verification by conductometric measurement). (b) Determination of solubility of a given salt at different temperature and plot solubility curve. (c) Determination of water of crystallisation of hydrated salt by ignition and weighing. **Group B** (a) Determination of the melting points of organic compounds (here, the student is required to learn about thermometer calibration before performing the experiment). (b) Effect of impurities on the melting point – mixed melting point of two unknown organic compounds. (c) Purification of organic compounds by crystallization using the following solvents: (a) water, (b) alcohol, (c) alcohol-water mixture. **Group C** (a) Evaluating the compressibility factor using standard packages such as Excel/Origin/Python/Fortran. (b) Simulating an ideal gas using programming. (c) Simulation of a real gas using programming. (d) To determine the partial molar volume of ethanol-water mixture at a given composition. (e) Determine the surface tension of a given liquid at room temperature using stalagmometer by drop number method. (f) Determine the surface tension of a given liquid by means of stalagmometer using drop weight method. (g) Determine the composition of a given mixture by surface tension method. (h) Study the variation of surface tension of detergent solutions with concentration. (*Students are required to perform Exp. 1, 2 and a minimum of two experiments from each group*)	30

Text Book /Reference Book	1. University Chemistry, P. Siska, O. K. Medhi, 2nd edition, Pearson Education 2. General and Inorganic Chemistry, R.P. Sarkar (part 1) 3rd edition, NCBA 3. Concise Inorganic Chemistry, J. D. Lee, 5th Edition, Pearson Education 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. Principles of Physical Chemistry, Puri, Sharma, Pathania, 48th Edition, Vishal Publishing Com. 6. Atkins Physical Chemistry, Atkins, de Paula and Keeler, 11th Edition, Oxford University Press. 7. Stereochemistry of Organic Compounds, D. Nasipuri, 4th Edition. 8. Reaction Mechanism in Organic Chemistry, S. M. Mukherji, S. P. Singh,3rd Edition. 9. Organic Reactions and their Mechanisms, P. S. Kalsi, 5th Edition. Solomons' Organic Chemistry, T. W. G. Solomons, C. B. Fryhle, S. A. Snyder.