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):

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

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

Unit I: Chemical bonding II (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. 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: 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: 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: 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

Unit V: Thermodynamics	Mathematical treatment: exact and inexact differentials, partial derivatives, Euler's reciprocity, cyclic rules. 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, ΔU and ΔH for expansion of ideal gas under isothermal and adiabatic conditions for reversible and irreversible processes. Derivation of Joule-Thomson coefficient and inversion temperature. 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 ΔH and ΔU of a reaction. Difference between enthalpy and standard enthalpy. 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.	15

Laboratory Course II	1. Preparation of buffer solution and measurement of pH using pH-meter (acetic acid-sodium acetate buffer) **Group A:** (a) Determination of total hardness of water by titration against standardised EDTA solution. (b) Synthesis of coordination compounds i) Potassium tris(oxalato)chromate(III), ii) $[Ni(DMG)_2]$ **Group B:** (a) Qualitative organic analysis for N, S and halogenin a given organic compounds. (b) Detection of presence of unsaturation and aromaticity in an organic sample. (c) Identify acidic functional groups of a given organic sample (Acetic acid, Lactic acid, Tartaric acid and Phthalic acid) and determine the pKa by titrametric methods. **Group C:** (a) Determination of heat capacity of a calorimeter and enthalpy of neutralisation (eg. hydrochloric acid with sodium hydroxide). (b) Determine the enthalpy of solution of oxalic acid from solubility measurements. (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). (d) Calculation of ionization enthalpy of ethanoic acid. (e) Determination of enthalpy of hydration of copper sulphate. *(Students are required to perform Exp. 1 and minimum of two from each group)*	30
Text Book /Reference Book	1. General and Inorganic Chemistry, R.P. Sarkar (part 1) 3rd edition, NCBA 2. Concise Coordination Chemistry, R. Gopalan, V. Ramalingam, 1st edition, Vikash Publishing House 3. Inorganic Chemistry (Principles of Structure and Reactivity), J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 5th edition, Pearson Education 4. Principles of Physical Chemistry, Puri, Sharma, Pathania, 48th edition, Vishal Publishing Com. 5. Atkins Physical Chemistry, Atkins, de Paula and Keeler, 11th edition, Oxford University Press. 6. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith 7th edition (Wiley). 7. Organic Chemistry, G. M. Loudon, 4th edition. 8. Mechanism and Theory in Organic Chemistry, Sachin Kumar Ghosh, New Central Book Agency.	