Established by Govt. of Arunachal Pradesh vide Act 9 of 2012, the Arunachal University of Studies Act, 2012 Recognized as per u/s 2(f) of University Grants Commission Act, 1956
NH-52, Namsai, Arunachal Pradesh -792103

MASTER OF SCIENCE (CHEMISTRY) – FIRST SEMESTER

First Semester			
S. No.	**Name of Subject**	**Credits**	**Total Marks**
1	Inorganic Chemistry – I	4	100
2	Organic Chemistry – I	4	100
3	Physical Chemistry – I	4	100
4	Green Chemistry	2	100
5	Analytical Chemistry - I	2	100
6	Lab-I	6	100
Total		**22**	

Subject: - Inorganic Chemistry - I

Course A: Stability constants of metal complexes and their applications

Stoichiometric and thermodynamic equilibrium constants, stepwise formation of complexes, formation functions, φ, n and $\propto$C and relationship between different functions. Calculation of stability constants. Graphical Methods: using sets of data {φ,[A]}; {$\propto C$,[A]} and {n,[A]}.

Curve fitting method, Elimination method, Numerical method, Potentiometric method. Method of corresponding solutions, Ion exchange method, Solvent extraction, Polarographic method, and Spectrophotometric methods which include Job's method of continuous variation, Logarithmic method. Bent and French mole ratio method. Turner and Anderson methods and Yatsimirskiis method.

Errors and Evaluation: Definition of the terms- mean and median, precision —standard deviation, relative standard deviation, accuracy-absolute error. Types of errors in experimental data determination (systematic), indeterminate (random) and gross. Sources of errors and their effect upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data -indeterminate errors. The use of statistics.

Analytical applications of complex formation; gravimetric analysis, complexometric titrations (Conditional constants, titration curves, titration error, detection of end point using metal indicators and instrumental methods. Indicator errors, Indicator correction etc. Simultaneous titrations, stepwise titrations, back titrations). Use of masking and demasking agents in complexometric titrations.

Course B: Supramolecular and Photoinorganic Chemistry

Molecular recognition: Receptors, design and synthesis of co-receptors and multiple recognition, Hydrogen bonds, strong, weak and very weak H-bonds, Utilisation of H-bonds to create supramolecular structures, Use of H-bonds in crystal engineering and molecular recognition, Chelate and macrocyclic effects.

Cation binding hosts, binding of anions, binding of neutral molecules, binding of organic molecules.

Supramolecular reactivity and catalysis. Transport processes and carrier design. Supramolecular devices, supramolecular photochemistry.
Redox reactions of metal complexes in excited states, excited electron transfer, examples using $[Ru(bpy)_3]^{2+}$ complex and $[Fe(bpy)_3]^{2+}$ complex. Role of spin-orbit coupling, lifetimes of excited states in these complexes.
Metal complex sensitizers: Electron relay, semiconductor supported metal oxide systems, water-photolysis, nitrogen fixation and CO_2 reduction.
Recommended Texts:

1. Inczedy, J. Analytical applications of complex equilibria Halsted Press: New York, NY (1976)..
2. Martell, A. E. & Calvin, M. Chemistry of the Metal Chelate Compounds. Prentice-HalI : N. Y. (1952).
3. Ringbom, A. Complexation in Analytical Chemistry Wiley: New York (1963).
4. Hartley, F. R. , Burgess, C. & Alcock. , R. M. Solution Equilibria Prentice-HalI : Europe (1980).
5. Beck, M. T. Chemistry of Complex Equilibria van Nostrand Reinhold: New York (1970).
6. Rossotti, F. J. C. & Rossotti, H. The Determination of Stability Constants McGraw Hill: London (1961).
7. Lippard, S.J. Progress in Inorganic Chemistry, Vol. 18, 3rd Ed. Wiley-Interscience (1991).
8. Lehn, J. M. Supramolecular Chemistry: Concepts & Perspectives Wiley-VCH (1995)..
9. Balzani, V. Photochemistry of Coordination Compounds Academic Press (1970)..
10. Desiraju, G. R. , Ed. Perspectives in Supramolecular Chemistry, Vol.2: Crystal Engineering and Molecular Recognition Wiley: Chichester (1995).
11. Atwood, J. L. & Steed, J. W. Supramolecular Chemistry: A Concise Introduction John Wiley & Sons (2000).
12. Adamson, A. W. & Fleischauer, P. D. (Eds.) Concepts of Inorganic Photochemistry, Wiley: New York (1975).

Subject: - Organic Chemistry - I

Course A: Organic Stereochemistry

Molecular symmetry and chirality: Symmetry operations and symmetry elements, point group classification and symmetry number.

Stereoisomerism: Classification, racemic modification, molecules with one, two or more chiral centres; Configuration nomenclature, D L, R S and E Z nomenclature. Axial and planar chirality and helicity (P & M); Stereochemistry and configurations of allenes, spiranes, alkylidine, cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes.
Topicity and prostereoisomerism: Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres.
Simple chemical correlation of configurations with examples, quasiracemates.
Cyclostereoisomerism: Configurations, conformations and stability of cyclohexanes (mono-, di- and tri-substituted) cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols and decalones.

Asymmetric induction: Cram's, Prelog's and Horeau's rules; Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, curtin-Hammett Principle.
Molecular dissymmetry and chiroptical properties. Linear and circularly polarised lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effect.The axial haloketone rule, octant diagrams, helicity, and Lowe's rule. Application of ORD and CD to structural and stereochemical problems.

Course B: Study of Reactive Intermediates
A review of reaction mechanisms including methods of determination.
Linear free energy relationships and their applications (Hammett equation and modifications).

Carbocations: Classical and non-classical, neighbouring group participation, ion-pairs, molecular rearrangements in acyclic, monocyclic and bicyclic systems, stability and reactivity of bridge-head carbocations.

Carbanions: Generation, structure and stability, ambident ions and their general reactions; HSAB principle and its applications.

Radicals: Generation, structure, stability and reactions, cage effects; radical-cations & radical-anions.

Carbenes: Formation and structure, reactions involving carbenes and carbenoids.

Nitrenes: Generation, structure and reactions of nitrenes.

Nucleophilic aromatic substituion; Benzynes, SNAr and SRN1 mechanisms; Ipso effect.

Recommended Texts:

1. Carey, F. A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (2004).
2. Eliel, E. L. Stereochemistry of Carbon Compounds Textbook Publishers (2003).
3. Finar, l. L. & Finar, A. L. Organic Chemistry,Vol. 2, Addison-Wesley (1998).
4. Finar, I. L. Organic Chemistry Vol. 1, Longman (1998).
5. Lowry. T. H. & Richardson, K. S. Mechanism and theory in Organic Chemistry Addison-Wes!ey Educational Publishers, Inc. (1981).
6. Nasipuri, D. N. Stereochemistry of Organic Compounds: Principles & Applications South Asia Books (1994).
7. March, J. Advanced Organic Chemistry John Wiley & Sons (1992).

Subject: Physical Chemistry-I

Quantum Chemistry

Postulates of quantum mechanics, Linear and Hermitian operators, Commutation of operators and Uncertainty Principle.

Differential equations, partial differential equations, series solutions and special functions, linear vector spaces, transformation of coordinate matrix, representation of operators, eigen value problem orthonormal sets, Fourier and Laplace transforms.

Some exactly soluble problems: Particle in a box and ring, Concept of degeneracy and Jahn-Teller distortion.

Simple harmonic oscillator problem and its solution using series solution or factorization method. Calculation of various average values using ladder operators and recursion relations of Hermite polynomials.

Angular momentum operators, Eigenvalues and eigen functions, Ladder operators, rigid rotator and hydrogen atom: Complete solution, Radial distributions, Virial theorem.

Approximate methods: First order time-independent perturbation theory for non-degenerate states, Variation theorem and variational methods, Use of these methods illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, approximate functions for particle in a box and hydrogen atom).

Ground and excited state of helium atom. Pauli's Exclusion principle. Many-electron atoms. Concept of spin and determinantal wave functions. Qualitative treatment of Hartree theory and Hartree-Fock SCF procedure.

Chemical bonding: Born-Oppenheimer approximation. Variational treatment of hydrogen molecule ion. Valence bond and MO (LCAO) treatment of hydrogen molecule. Comparison of the MO and VB treatments

and their equivalence limit. Configuration Interaction. Extension of MO theory to other systems- Homonuclear and heteronuclear diatomics, polyatomics. Walsh diagrams for dihydrides, linear and bent triatomics.

HMO method and its applications: π-Electron approximation, Hückel Molecular Orbital Theory of conjugated systems. Calculation of properties- Delocalization energy, electron density, bond order, alternant and nonalternant hydrocarbons. Pairing theorem. Electronic and ESR spectra. Effect of substituents on spectra. Reactivity and electrocyclic ring closures.

Recommended Texts:

1. Lowe, J. P. & Peterson, K. Quantum Chemistry Academic Press (2005).
2. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt. Ltd.: New Delhi (2003).
3. Mortimer, R. G. Mathematics for Physical Chemistry 2nd Ed. Elsevier (2005).
4. Pilar, F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (200 1).
5. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
6. Levine, I. L. Quantum Chemistry 5th Ed, Prentice-Hall Inc.: New Jersey (2000).
7. Engel, T. & Reid, P. Physical Chemistry Benjamin-Cummings (2005).
8. McQuarrie, D. A. & Simon, J. D Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books (2001).
9. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed. Wiley (2004).

Subject: - Green Chemistry

Introduction to Green Chemistry
The need of Green Chemistry, principles of Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry

Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products , Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.

Prevention/ minimization of hazardous/ toxic products reducing toxicity. risk = (function) Hazard × exposure; waste or pollution prevention hierarchy. Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents.

Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy. Selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups.

Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.

Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD "What you don't have cannot harm you", greener alternative to Bhopal Gas Tragedy (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation. Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co crystal controlled solid state synthesis (C2S3); Green chemistry in sustainable development.

Recommended Texts:

1. Ahluwalia, V.K. & Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers (2005).
2. Anastas, P.T. & Warner, J.K.: Green Chemistry - Theory and Practical, Oxford University Press (1998).
3. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
4. Cann, M.C. & Connely, M.E. Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
5. Ryan, M.A. & Tinnesand, M. Introduction to Green Chemistry, American Chemical Society, Washington (2002).
6. Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2nd Edition, 2010.

Subject: - Analytical Chemistry - I

Introduction: Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. Presentation of experimental data and results, from the point of view of significant figures.

Analysis of soil: Composition of soil, Concept of pH and pH measurement, Complexometric titrations, Chelation, Chelating agents, use of indicators

(a) Determination of pH of soil samples.

(b) Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

Analysis of water: Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.
(a) Determination of pH, acidity and alkalinity of a water sample.
(b) Determination of dissolved oxygen (DO) of a water sample.

Analysis of food products*:* Nutritional value of foods, idea about food processing and food preservations and adulteration.
(a) Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
(b) Analysis of preservatives and colouring matter.

Chromatography: Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.
(a) Paper chromatographic separation of mixture of metal ion (Fe^{3+} and Al^{3+}).
(b) To compare paint samples by TLC method. Ion-exchange: Column, ion-exchange chromatography etc. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Analysis of cosmetics: Major and minor constituents and their function
(a) Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.
(b) Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

Recommended Texts:

1. Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. Instrumental Methods of Analysis. 7th Ed. Wadsworth Publishing Co. Ltd., Belmont, California, USA, 1988.
2. Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis, Cengage Learning India Ed.
3. Skoog, D.A.; West, D.M. & Holler, F.J. Fundamentals of Analytical Chemistry 6th Ed., Saunders College Publishing, Fort Worth (1992).
4. Harris, D. C. Quantitative Chemical Analysis, W. H. Freeman.
5. Dean, J. A. Analytical Chemistry Notebook, McGraw Hill.
6. Day, R. A. & Underwood, A. L. Quantitative Analysis, Prentice Hall of India.
7. Freifelder, D. Physical Biochemistry 2nd Ed., W.H. Freeman and Co., N.Y. USA (1982).
8. Cooper, T.G. The Tools of Biochemistry, John Wiley and Sons, N.Y. USA. 16 (1977).
9. Vogel, A. I. Vogel's Qualitative Inorganic Analysis 7th Ed., Prentice Hall.
10. Vogel, A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Prentice Hall.
11. Robinson, J.W. Undergraduate Instrumental Analysis 5th Ed., Marcel Dekker, Inc., New York (1995).