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) – SECOND SEMESTER

Second Semester			
S. No.	**Name of Subject**	**Credits**	**Total Marks**
1	Inorganic Chemistry - II	4	100
2	Organic Chemistry - II	4	100
3	Physical Chemistry - II	4	100
4	Retro Synthesis	2	100
5	Analytical Chemistry II	2	100
6	Lab-II	6	100
Total		**22**	

Subject: - Inorganic Chemistry – II

Course A: Group Theory and its Applications

Molecular symmetry: Symmetry elements and symmetry operations, definition of group and its characteristics, subgroups, classes, similarity transformation.

Products of symmetry operations, equivalent atoms and equivalent symmetry elements , relations between symmetry elements and operations, classes of symmetry operations. Point groups and classification.

Symmetry: Optical activity and dipole moment.

Representation of groups. Reducible and irreducible representations. The Great Orthogonality theorem. Character tables, position vector and base vector as basis for representation.

Wavefunctions as bases for irreducible representations (p- and d-orbitals). Direct product .Vanishing integral.

Russell-Saunders coupling for dn states. Splitting of one-electron levels in an octahedral environment. Correlation diagram. The method of descending symmetry, selection rules.

Spectral transition probability, vibronic coupling. Non-centrosymmetric complexes. Polarization of allowed transitions.

Symmetry: Infrared and Raman Spectroscopy.

SALCs, projection operators. Illustrative examples.

Hybridization and its applications. Hybrid orbitals as Linear Combinations of Atomic Orbitals. Selected examples. MOs using Group Theory principles

Symmetry and chemical reactions.

Course B: Chemistry of d-and f-block elements :

Term-symbols, Russel-Saunders states. Crystal field theory and splitting in Oh, Td, D4h and C4v systems, Orgel and Tanabe-Sugano diagrams, determination of Dq and Racah parameters, oxidation states and electronic absorption spectra of complex ions. Spectrochemical series and effects of covalency, nephelauxetic series, magnetic properties of transition metal complexes and lanthanides, metal-metal bonds, cluster compounds of d-block elements. poly-oxo metallates of Ru, Os, Mo. Structure and bonding in complexes containing π-acceptor ligands. Relativistic effects affecting the properties of heavier transition elements..

Recommended Texts:

1. Cotton, F. A. Chemical Applications of Group Theory Wiley Interscience: N.Y (1990).
2. Jaffe, H. H. & Orchin. M. Symmetry in Chemistry Dover Publications (2002).
3. Hatfield, W. F. & Palmer, R. A. Problems in Structural Inorganic Chemistry W. A. Benjamin, Inc .:NY (1971) .
4. Hatfield. W. E. & Parker, W. E. Symmetry in Chemical Bonding & Structure C. E. Merrill Publishing co.: USA (1974).
5. Bishop, D. M. Group Theory and Chemistry, Clarendon Press: Oxford, U.K. (1973).
6. Shriver, D. F., Atkins, P. W. & Langford, C. H. Inorganic Chemistry, 2nd Ed., Oxford Univ. Press (1998)
7. Purcell. K. F. & Kotz. J, C Inorganic Chemistry. W B. Saunders and Co.: N. Y. (1985).
8. Wulfsberg, G. Inorganic Chemistry Univ. Science books: USA (2000); Viva Books: New Delhi.
9. Sutton, D. Electronic Spectra of Transition Metal Complexes McGraw-Hill.' New York (1968).
10. Mabbs. F. E. & Machin. D. J. Magnetism and Transition Meta/ Complexes Chapman and Hall : U.K. (1 973).
11. Drago, R. S. Physical Methods in Chemistry, W. B. Saunders Co.: U.K. (1977).

Subject – Organic Chemistry – II

Course A: Spectroscopy

PMR: Natural abundance of 13C, 19F and 31P nuclei; the spinning nucleus, effect of external magnetic field. precessional motion and frequency, Energy transitions, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect; Integrals of protons. Spin-spin coupling, splitting theory. Magnitude of coupling constant; Simple, virtual and complex spin-spin coupling; Chemical and magnetic equivalence. Proton exchange, factors affecting the coupling - First and non-first order spectra; Simplification of complex spectra (solvent effect, field effect, double resonance and lanthanide shift reagents) and NOE experiments (NOESY, HOESY, ROESY, etc.). Applications of PMR in structural elucidation of simple and complex compounds.

CMR: Resolution and multiplicity of 13C NMR. 1H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR. DEPT and INEPT experiments; Introduction to 2D-NMR; COSY, HMQC and HETEROR spectra.
ESR: Derivative curves, hyperfine splitting, g-values, ESR spectra of simple molecules.

MASS: Theory, instrumentation and modifications; Unit mass and molecular ions; Important terms- singly. doubly/multiple charged ions, metastable peak, base peak, isotopic mass peaks, relative intensity, FTMS, etc.; Recognition of M+ ion peak; Ionization methods (El, CI and FAB), General fragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulphur, nitrogen and halogens; α-,β-, allylic and benzylic cleavage; McLafferty rearrangement; ESI, APCI and MALDI, etc.
Combined problems on UV, IR, NMR and MASS

Course B: Methods in Organic Synthesis

Organosilicone Compounds: Preparation and applications in organic synthesis; Applications of Pd(0) and Pd(II) complexes in organic synthesis- Stille, Suzuki and Sonogashira coupling, Heck reaction and Negishi coupling.

Preparation and applications of lithium organocuparates.
Reductions: Stereochemistry, stereoselection and mechanism of catalytic hydrogenation and metal-liquid ammonia reductions.

Hydride transfer reagents: Sodium borohydride, sodium cyanoborohydride, lithium aluminium hydride and alkoxy substituted LAH reducing agents, DIBAL; Applications of hydroboration (reductions, oxidations and cabonylations): diborane, diisoamylborane, thexylborane, 9-BBN, isopinocamphenyl and diisopinocamphenyl borane.

Homogeneous hydrogenations: Mechanisms and applications using Rh, Ru and other metal complexes.
Oxidations: Scope of the following oxidising reagents with relevant applications and mechanisms: DDQ, SeO_2, $Tl(NO_3)_3$ Sharpless epoxidation.

Recommended Texts:
1. Carruthers, W. Modern Methods of Organic Synthesis Cambridge University Press (1971).
2. Kemp. W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co. (1991).
3. Silverstein, R M., Bassler, G. C & Morrill, T. C. Spectroscopic Identification of Organic Compounds John Wiley & Sons (1981).
4. March, J. Advanced Organic Chemistry John Wiley & Sons (1992).

Subject: - Physical Chemistry-II

Statistical mechanics and thermodynamics*:*

Fundamentals: Concept of distribution. Thermodynamic probability and most probable distribution. Canonical and other ensembles. Statistical mechanics for systems of independent particles and its importance in chemistry. Types of statistics: Maxwell-Boltzmann. Bose-Einstein and Fermi-Dirac statistics. Idea of microstates and macrostates. Thermodynamic probability (W) for the three types of statistics. Derivation of distribution laws (most probable distribution) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance. Assembly partition function.

Applications to ideal gases: The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases. The electronic and nuclear partition functions. Calculation of thermodynamic properties of ideal gases in terms of partition function. Statistical definition of entropy. Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number. Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures.
Einstein theory and Debye theory of heat capacities of monatomic solids.
Third law of thermodynamics, Residual entropy.
Electrochemistry: Solutions: Activity coefficients and ion-ion interactions. Physical significance of activity coefficients, mean activity coefficient of an electrolyte and its determination. Derivation of the Debye-Huckel theory of activity coefficients (both point ion size and finite ion size models). Excess functions.

Kinetics:
Theories of reaction rates: Collision theory. Potential energy surfaces (basic idea). Transition state theory (both thermodynamic and statistical mechanics formulations). Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment).
Solution kinetics: Factors affecting reaction rates in solution. Effect of solvent and ionic strength (primary salt effect) on the rate constant. Secondary salt effects.

Macromolecules: Concepts of number average and mass average molecular weights. Methods of determining molecular weights (osmometry, viscometry, sedimentation equilibrium methods). Theta state of polymers. Distribution of chain lengths. Average end-to-end distance.

Recommended Texts:
1. McQuarrie, D. A. Statistical Mechanics Viva Books Pvt. Ltd.: New Delhi (2003).
2. Nash, L. K. Elements of Statistical Thermodynamics, 2nd Ed., Addison Wesley ( ] 974).
3. Laidler. K. J. Chemical kinetics 3rd Ed., Benjamin Cummings (1997).
4. Billmeyer. F.W. Textbook of Polymer Science 3rd Ed. Wiley-Interscience: New York (1984).
5. Atkins. P. W. & Paula. J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
6. McQuarrie. D. A. & Simon. J. D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books

Subject: - Retro Synthesis

Introduction: General Aspects of Retrosynthetic Analysis, Disconnection Versus Interconversion of the Functional Group, Retrosynthesis and Asymmetric Synthesis, Interconversion of Functional Groups, and C–H Acidity. Interconversions of Oxygenated Functional Groups, Acidity of C–H Bond, Stabilization of Carbanions, Organic Synthesis and the Environment

Retrosynthetic Analysis of the Compounds with One Functional Group: Disconnection of Carbinols, Disconnection of Alkenes, Examples of the Wittig Reaction on the Industrial Scale, Disconnection of

Ketones, Disconnection of Dialkyl Ketones, Alkyl Aryl Ketones and Diaryl Ketones, Interconversion of the Nitro Group, Nitroalkanes as Building Blocks

Stereoisomers and Stereoselective Reactions: ["Departure into Third Dimension"]: Retrosynthesis and Stereochemical Aspects of Synthetic Reactions, Basics of Stereoselective Reactions, Topological Relation and Stereoselectivity, Stereoselective Processes and Kinetic Control, Reaction Stereochemistry, More About Enantioand Diastereoselectivity, Examples of Asymmetric Syntheses, Hydrogenation of the C=O Bond Catalyzed by Chiral Organometallic Complexes, Hydrogenation of the C=N Bond Catalyzed by Chiral Organometallic Complexes, Asymmetric Alkylation of Stabilized Carbanion

Disconnection with Participation of Two Functional Groups: Match and Mismatch of Charges in Bifunctional Molecules, 4.3 1,3-Dioxygenated Pattern (1,3-CO), 1,3-Hydroxycarbonyl Compounds, 1,3-Dicarbonyl Compounds, Concept of Hard and Soft Acids and Bases (HSAB), 1,5-Dicarbonyl Pattern (1,5-CO), From Retrosynthesis to Robinson Annulation, Vinyl Ketones via the Mannich Reaction.

Illogical Disconnections with Participation of Two Groups: 1,2-Dioxygenated Pattern (1,2-CO), Illogical Nucleophiles, Three-Membered Heterocyclic Rings, Illogical Electrophiles, 1,2-Dihidroxy Pattern, Vicinal Diols, 1,4-Dioxygenated Pattern (1,4-CO), 1,4-Dicarbonyl Compounds, 1,4-Hydroxy Carbonyl Compounds. 1,6-Dicarbonyl Pattern (1,6-CO)

Recommended Texts:]

1. Stuart Warren, Organic synthesis, the disconnection approach, John Wiley & sons, 1992.
2. Vitomir Sunjic, Vesna Petrovik, Organic Chemistry from Retrosynthesis to Asymmetric Synthesis, Springer, 2015
3. Carey FA, Sundberg RJ (2007) Advanced organic chemistry. Part B. Reactions and synthesis, 5th edn. Springer, Berlin
4. Smith JG (2011) Organic chemistry, the Diels-Alder reaction, 3rd edn. McGraw-Hill, New York

Subject: - Analytical Chemistry II

X-ray Diffraction: Principles and applications of powder and single crystal X-ray Diffraction (XRD)

Thermal methods: Principles and application of Thermogravimetry (TG), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC)

Surface Science: Adsorption and Desorption isotherms, Particle size analysis (PSA) and Pore size distribution (PSD)

Chromatography: Gas Chromatography (GC) and High Performance Liquid Chromatography (HPLC)

Electron Microscopy: Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM)

Recommended Texts:

1. Instrumental Methods of Chemical Analysis - H Kaur, Pragati Prakashan
2. Introduction to Thermal Analysis: Techniques and Applications - M.E. Brown, Springer
3. Introduction to instrumental Analysis - R.D. Braun, McGraw Hill.