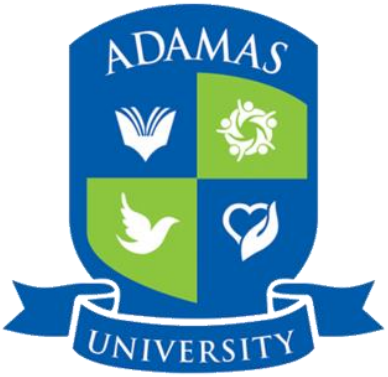
Course Curriculum

MASTER OF SCIENCE

IN CHEMISTRY



ADAMAS UNIVERSITY

Barasat, Kolkaa-126

M.Sc. in Chemistry
Adamas University
Syllabus

Semester I

Physical Chemistry I (45L) **CHM21080**

Unit 1: Classical Thermodynamics (12L)

Concepts involved in first, second and third law of thermodynamic, Thermodynamic equation of state, Maxwell relations, Free energy and entropy of mixing, Partial molar quantities, Gibbs-Duhem equation. Equilibrium constant, Temperature-dependence of equilibrium constant. Ideal and non-ideal solutions, Activity and activity coefficient, Mean ionic activity coefficient, Ionic strength, Determination of activity and activity coefficient by Debye Hückel law, Concept of fugacity and determination of fugacity.

Unit 2: Interfacial Chemistry and Micelles (8L)

Effects of confinement and finite size; Concepts of surface and interfacial energies and tensions; Apolar (van der Waals) and polar (acid-base) components of interfacial tensions Young-Laplace equation of capillarity; examples of equilibrium surfaces; multiplicity, etc. Micelles, reverse micelles; micellization equilibrium; thermodynamics of micellization; micro- and macro- emulsions, applications of micelles and reverse micelles

Unit 3: Chemical Kinetics (12L)

Collision theory, modified collision theory; weakness of the collision theory, transition state theory; potential energy surface (a concept); equilibrium, Hypothesis, primary and secondary kinetic isotope effect; Fast reactions; Relaxation method, fast photolysis. Chain reaction, explosion; oscillatory reaction (Belousov -Zhabotinsky reaction); unimolecular reaction (Lindemann - Hinshelwood and Rice-Ramsperger -Kassel-Marcus [RRKM] theories of unimolecular reactions).

Unit-4: Electrochemistry (13)

Thermodynamics of reversible electrodes and reversible cells. Zeta potential, OHP and IHP, potential profile across double layer region, potential difference across electrified interface; structure of the double layer: Helmholtz-Perrin, Gouy-Chapman, and Stern models. Redox indicators, Debye-Hückel treatment of dilute electrolyte solutions, Derivation of Debye-Hückel limiting law, Extended Debye-Hückel law, Debye-Hückel length. Photoelectrochemical cells. Butler-Volmer equation under near equilibrium and nonequilibrium conditions, exchange current density, Tafel plot, polarizable and non-polarizable interfaces.

Reference Books:

1. The Principles of Chemical Equilibrium – K. Denbigh
2. Micelles: Theoretical and Applied Aspects, Y. Moroi, Plenum Press, New York (1992).
3. Physical Chemistry, 8 th edition, P.W. Atkins
4. Thermodynamics for Chemist, S. Glasstone, D. Van Nostrand, 1965.
5. Chemical Kinetics, K. J. Laidler, McGraw Hill, 1985.
6. Kinetics and Mechanism, Frost and Pearson
7. Physical Chemistry, G. W. Castellan, AddisionWeslay
8. Modern Electrochemistry, Vol. 2 A & B, J.O'M. Bockris and A. K. N. Reddy, 2nd Ed.
1. Plenum Press, New York
9. An Introduction to electrochemistry, S. Glasstone.

Inorganic Chemistry I (45L) **CHM21081**

Unit-1: Bonding in Transition Metal Complexes (30 L)

Crystal field theory, Splitting of d orbitals in tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral fields of similar and dissimilar ligands. Crystal field stabilization energies in weak field and strong field environments, octahedral site preference energy, tetragonal distortion and Jahn Teller effect. Shapes of complexes. Effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy and stability of complexes (Irving Williams order). MO energy diagram for octahedral ML6, tetrahedral ML4 and square planar ML4 complexes with sigma-only donor ligands; MO energy diagram for octahedral ML6 and tetrahedral ML4 complexes with pi donor/ pi-acceptor ligands.

Unit-2: Electronic spectra of transition metal complexes (15 L)

Determination of free ion terms of d^1 to d^9, microstates, determination of ground and all excited state terms of d^n terms in octahedral and tetrahedral fields, Orgel diagrams (qualitative approach), hole formalism, inversion and equivalence relations, selection rules for spectral transitions, d-d spectra and crystal field parameters, Nephelauxetic series, qualitative idea of Tanabe–Sugano diagrams, charge transfer spectra. Definition of magnetic properties, Curie and Curie-Weiss Law, Orbital and spin contribution to magnetic susceptibility, Introduction to magnetic properties to Lanthanides, Magnetic exchange coupling, Spin-cross over phenomena.

Reference Books

1. Douglas, B.E. and McDaniel, D.H. *Concepts & Models of Inorganic Chemistry* Oxford, 1970
2. Shriver and Atkins, *Inorganic chemistry*
3. Huheey, Keiter and Keiter, *Principles of Inorganic Chemistry*
1. 4.Cotton, F. A., *Chemical Applications of Group theory*
4. Jaffe, H. H., *Symmetry in Chemistry*

Organic Chemistry I (45L) **CHM21082**

Unit-I: Stereochemistry **(20L)**

Static Aspects: Symmetry properties, point group, configuration – acyclic and cyclic systems; conformation – cyclic systems (Cyclopropane, Cyclobutane, Cyclopentane, substituted cyclopentanes and cyclopentanones, Cyclohexane, cyclohexene, cyclohexanone, medium rings, decalin, hydrindane systems, perhydrophenanthrenes, perhydroanthracenes).

Dynamic Aspects: Conformation and reactivity with reference to substitution, elimination, addition, rearrangement reactions, cyclisation reactions, Baldwin‘s Rules with example; Curtin-Hammett Principle, Zimmerman Traxler model for Aldol reaction.

Unit-II: Pericyclic Reaction **(25L)**

Pericyclic reactions: Molecular orbitals for acyclic conjugated systems. Theory of pericyclic reactions – i) Frontier Molecular Orbital (FMO) approach ii) concept of aromaticity of transition states (Hückel/ Möbius systems). The Woodward-Hoffmann selection rules and general rules. General perturbation molecular orbital theory in cycloadditions: Symmetry principles in pericyclic reactions, orbital and state correlation diagram for electrocyclic and cycloaddition reactions. Reactivity, regioselectivity and periselectivity. Cycloaddition reactions: antarafacial and suprafacial additions, 4n and 4n+2 systems; 2,2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Transannular effect in Diels-Alder reaction. Ene reactions, group-transfer reactions and eliminations. Scope, reactivity and stereochemical features of electrocyclic reactions (4e, 6e and 8e neutral systems). Electrocyclic reactions of charged systems (cations and anions), Electrocyclic reactions: conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Sigmatropic rearrangements: [1, j] shifts – [1, 5] and [1, 7] shifts in neutral systems and [1,4] shift in charged species: [I, j] shifts – [3, 3] shifts, Sommelet-Hauser, Cope, aza-Cope rearrangements, Fluxional tautomerism. Claisen rearrangements; [5, 5] shifts, [2, 3] shifts in ylids.

Reference Books:

1. Stereochemistry of Organic Compounds – E. L. Eliel and S. H. Wilen.
2. Stereochemistry of Organic Compounds – D. Nasipuri.
3. Pericyclic Chemistry – S. M. Mukherjee.
4. Frontier Orbitals and Organic Chemical Reactions – I. Fleming

Mathematical and Computational Chemistry **CHM23129**

Unit-I: Mathematics-I **(15)**

Numbers, functions, Extremum principles, constrained extremization, Power series: Convergence and divergence, Taylor series and Fourier series. Vectors and linear vector space: matrices and determinant.

Unit-II: Probability and statistics **(5)**

Probability distribution function, variance, standard deviation, error analysis: systematic and random error, linear regression model, correlation analysis.

Unit-III: Numerical analysis (15)

Roots of equations: Quadratic formula, iterative method, Newton-Raphson method, Numerical differentiation, Numerical integration (Trapezoidal and Simpson's rule), Simultaneous equations: Gauss elimination Matrix: Gauss-Siedal method, Monte Carlo methods, Differential equation: Euler and Rung-Kutta method.

Unit-IV: FORTRAN programming (10)

Computer programming in FORTRAN. Syntax for formula translation, Decision making statement, loop, array, subroutine.

Reference Books:

1. Fortran77 and Numerical Methods, C Xavier, New Age International (P) Ltd.
2. Modern Fortran in Practice, Arjen Markus, Cambridge Univrsity Press (2012).
3. Numerical Recipe in Fortran77, The art of scientific computing. W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, 2nd Edition, Cambridge Univrsity Press.
4. Mathematics for Chemists, N. K. Bera, S. Ghosh, P. Ghosh. TechnoWorld.

Corresponding Lab:

A. General Programming:

1. Summation of the terms of series
2. Swapping and sorting
3. Integration, differentiation
4. Plotting straight line.
5. Finding correlation coefficient
6. Extrapolation, interpolation
7. Matrix operations
8. Differential equation

B. Application to Chemical problems:

Chemical Kinetics, Quantum mechanics, Statistical Thermodynamics etc.

Reference Books:

1. Fortran77 and Numerical Methods, C Xavier, New Age International (P) Ltd.
2. Modern Fortran in Practice, Arjen Markus, Cambridge Univrsity Press (2012).
3. Numerical Recipe in Fortran77, The art of scientific computing. W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, 2nd Edition, Cambridge Univrsity Press.
4. Mathematics for Chemists, N. K. Bera, S. Ghosh, P. Ghosh. TechnoWorld.
5. Quantum Chemistry, I. N. Levine, Prentice Hall.

Analytical Chemistry (30L) **CHM21083**

Unit-I: Analytical Chemometrics (5 L)

Propagation of measurement uncertainties (inaccuracy and imprecision). Useful statistical test: test of significance, the F test, the student 't' test, the chi-test, the correlation coefficient, confidence limit of the mean, comparison of two standard values, comparison of standard deviation with average deviation.

Unit-II: Analytical tools for Characterization of Complexes (15 L)

Introduction to spectrometric methods and components of optical instruments. Atomic absorption, fluorescence, mass, and X-ray spectrometry. Introduction and applications of UV-vis molecular absorption, luminescence, infrared, Raman, nuclear magnetic resonance, and mass spectroscopy/ spectrometry

Unit-III: Separation Methods: (10L)

Principle of chromatography, Classifications of chromatography, Techniques of planar and column chromatography, Gas chromatography, High-performance liquid chromatography

Reference Books:

1. Vogel, Arthur I: *A Text book of Quantitative Inorganic Analysis*
2. Christian, Gary D; *Analytical Chemistry*
3. Khopkar, S.M., *Basic Concepts of Analytical Chemistry*.
4. Mukherjee, G. N., *Advanced Experiments in Inorganic Chemistry*

Physical Chemistry Lab **CHM22084**

A. Spectrophotometric study:

1. To test the validity of Beer-Lambert's law and hence determination of unknown concentration in a solution
2. Iodination of Acetone: Study of the kinetics of zero order reaction.
3. Study the effect of ionic strength on the reaction: $K_2S_2O_8 + KI \rightarrow 2K_2SO_4 + I_2$; spectrophotometrically.
4. Autocatalytic reaction: reaction of $KMnO_4$ with oxalic acid

B. Conductometric study:

1. Determination of CMC
2. To determine the basicity of a polybasic acid and its dissociation constant.
3. Titration of mixed halide ($KCl+HCl+NH_4Cl$) by $AgNO_3$

C. Determination of the value of Plank's constant

D. Kinetic study with polarimeter

1. Acid catalysed mutarotation; effect of acid concentration, effect of different acids.

Reference Books:

1. Findlays Practical Chemistry, Revised by J. A. Kitcher.
2. Text Book of Quantitative Inorganic Analysis, by A. I. Vogel.
3. Experimental Physical Chemistry, by R. C. Das and Behera.
4. Advanced Practical Physical Chemistry, by J. B. Yadav, Goel Publishing.
5. Experimental Physical Chemistry, by F. Daniels and J. Williams.

Inorganic Chemistry Lab **CHM22085**

Course Content

1. Spectrophotometric, ion exchange and complexometric estimations.
2. Qualitative analysis of mixture of compounds containing two rare elements and insoluble samples
3. Rare elements: Ti, V, Mo, W, Zr, Ce, U
4. Insoluble Samples: $PbSO_4$, $BaSO_4$, $SrSO_4$, Fe_2O_3, CaF_2, Cr_2O_3, Al_2O_3, SiO_2, SnO_2, TiO_2, ZrO_2, CeO_2

Reference Books

1. G. N. Mukherjee, *Handbook of Inorganic Analysis*
2. Arthur I Vogel, Qualitative Inorganic Analysis.

Semester II

Physical Chemistry II (45L) **CHM21087**

Unit-1: Quantum Mechanics-I (10)

Postulates and their analysis. Equation of motion. Stationary states, Quantization Schemes, Ehrenfest's theorems, free particle, Barrier problems and tunneling. Born-Oppenheimer (B.O.) approximation. Virial theorem and chemical bonding.

Unit-II: Quantum Mechanics -II (10)

Angular Momentum Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular momenta, Harmonic oscillator. H-atom Problem: Cartesian and polar coordinates. Centre of mass and relative coordinates. General forms of solutions and orbital specifications. Spherical harmonics. Real and complex orbitals. Role of constant motion.

Unit-II: Quantum Mechanics -III (3)

Approximation methods: Variational theorem; Time-independent Perturbation treatment (for nondegenerate systems).

Unit-III: Statistical Thermodynamics (12L)

Entropy and probability. Derivation of Maxwell-Boltzmann distribution. Relevance to thermodynamics. Rotational, Translational, Vibrational and Electronic partition function (PF) for diatomic molecules, Calculation of equilibrium constants in term of partition function. Theories of specific heat for solids. Application to chemical/ionization equilibrium, Equipartition principle. Gibbs paradox, and quantum statistics (preliminary idea). Third law and residual entropy.

Unit -IV Solid State Chemistry (10L)

General principles and experimental procedure of solid state reactions, growth of single crystals: Czochralski, Bridgman and Stockbarger methods. Defects and Non-stoichiometric - Intrinsic and extrinsic defects - point, line and plane defects; vacancies, Stoichiometric defects - Schottky and Frenkel defects - Non-stoichiometry – Metal excess and Metal-deficiency. Thermodynamic and structural aspects. n- And p- type semiconductors–photovoltaic cell – Superconductivity.

References:

1. West, A. R., Solid State Chemistry and Its Applications, John Wiley & Sons, 1984
2. Chakrabarty, K., Solid State Chemistry, New Age Publishers, 1996.
3. Quantum Chemistry, I.N. Levine, Pearson Educ., Inc. New Delhi.
1. 4.Introduction to Quantum Mechanics. D. J. Griffiths, Prentice Hall.
4. Statistical Mechanics, D. A. McQuarrie, Harper & Row

5. Introduction to Solid State Physics, C. Kittle. Wiley India.
6. Statistical Mechanics, R.K.Pathria, P.D.Beale, Elsevior.
7. Introduction to Quantum Mechanics – L. Pauling, E. B. Wilson

Inorganic Chemistry II (45L) CHM21088

Unit-I: Kinetics and Mechanism of Substitution Reactions (10 L)

Nature of substitution reactions; prediction of reactivity of octahedral, tetrahedral and square-planar complexes in terms of crystal field activation energy and structure preference energy; rates of reactions; acid hydrolysis, base hydrolysis and anation reactions.

Unit-II: Special aspects of s and p block elements (10 L)

Polyhedral boranes: Electron deficiency *vs* sufficiency. Types and IUPAC nomenclature. Wade's polyhedral skeleton electron pair theory (PSEPT). W. N. Lipscomb's *styx* rules and semi-topological structures of boranes. Equivalent and resonance structures. Carboranes, structure and bonding.

Metal Clusters: Metal-metal bonds. Concept of quadrupolar bond and its comparison with a C-C bond; Types of metal clusters and multiplicity of M-M bonds. Dirhenium complexes.

Unit-III: Chemistry of d and f-block elements (10 L)

Lanthanide and actinide elements: terrestrial abundance and distribution, relativistic effect, variation of atomic and ionic radius, ionization energy, electronic configuration and oxidation states, magnetic properties, electronic spectra, aqueous and complex chemistry in different oxidation states, comparison with those of d-block elements; organometallic compounds, use of lanthanide compounds as NMR-shift reagent and others. Super heavy elements.

Unit-IV: Organometallic Chemistry (15 L)

Preliminary idea and applications of 16 and 18 electrons rule for organometallic compounds. Preparation, structure, and properties: bonding in metal carbonyls, variants of CO bridging, vibrational spectra of metal carbonyls. Catalysis by organometallic compounds: Wilkinson's catalyst, Tolman's catalytic loops; synthesis gas, water gas shift reaction, synthesis of methanol, hydroformylation (oxo process), hydrogenation of unsaturated compounds, Monosanto acetic acid process, Wacker process, synthetic gasoline, Fischer-Tropsch process and mobil process; Polymerisation, oligomerisation and metathesis reactions of alkenes and alkynes; Zieglar-Natta catalysis.

Reference Books:

1. F. Basolo and R.C. Pearson, *Mechanisms of Inorganic Chemistry*
2. B. D. Gupta and A. J . Elias, *Organometallic Chemistry*

3. Greenwood, N.N. &Earnshaw. *Chemistry of the Elements*, Butterworth-Heinemann. 1997.
4. Cotton, F.A. & Wilkinson, G. *Advanced Inorganic Chemistry*, Wiley, VCH, 1999.
5. Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. *Concepts & Models of Inorganic Chemistry*

Organic Chemistry II (45L) CHM21089

UNIT-I: Synthetic strategy (25L)

Enolate chemistry: Enolates and enamines: formation; alkylation and acylation, reactions withcarbonyls, conjugate addition. Chemistry of acetoacetic ester and malonic ester. Strategy of ring synthesis: thermodynamic factor, synthesis through enolate anion chemistry and carbonyl condensation reactions (including acetoaceticester & malonic ester synthesis), synthesis through rearrangement (including pinacol, Favorski), synthesis of large rings, high dilution technique and acyloin reaction, Stobbe condensation.

Retrosynthetic analysis (disconnections, synthons, donor and acceptorsynthons,functional group interconversion, C-C disconnections and synthesis [one group and two group (1,2 to 1,6-dioxygenated], reconnection (1,6-di carbonyl), natural reactivity and umpolung, protection-deprotection strategy [alcohol, amine, carbonyl, acid], disconnection, typical examples to illustrate the disconnection approach to organic synthesis).

Unit-II: Heterocyclic Chemistry (20L)

Systematic nomenclature (Hantzsch–Widman system) for monocycle and fused heterocycles. General approach to heterocyclic synthesis–cyclisation and cycloadditionroutes. Heterocycles in organic synthesis – masked functionalities, umpolung, Stork annulation reaction and applications. Synthesis and reactivity of pyrrole, pyridine, quinoline, isoquinoline, indole, pyrazole, imidazole, oxazole, thiazole and their applications in organic synthesis. Rearrangement and ring transformation involving 5-and 6-membered heterocycles with one heteroatom**.** (synthesis of testosterone, estrone, progesterone, ranitidine, lansoprazole and/or recently discovered molecules etc.).

Reference Books:

1. Organic Synthesis - The Disconnection Approach – S. Warren
2. Designing Organic Synthesis – S. Warren
3. Tactics of Organic Synthesis - T.-L. Ho.
4. Exercise in Synthetic Organic Chemistry - C. Ghiron& R. J. Thomas.
5. Heterocyclic Chemistry - J. A. Joule & K. Mills.
6. Heterocycles in Synthesis – A. I. Meyers.

Group Theory and Spectroscopy (45L) CHM21090

Unit 1: Group Theory (20 L)

Introduction, symmetry elements and group theory, group theory and quantum mechanics (elementary ideas), reducible and irreducible representations of point group, definitions of classes and character, statement of grand orthogonality theorem, orthogonality theorem for characters, character tables, concept of character projection operator.
Selection rules in molecular spectroscopy, Vibration of polyatomic molecules – Normal modes, their symmetry properties, IR and Raman activity. Electronic spectroscopy, crystal field theory.SALC – Hückel theory, Hybridization, Vibronic coupling.

Unit-2 Rotational and rotation-vibrational spectroscopy (15 L)

Microwave and Infrared spectroscopy of di- and polyatomic molecules (symmetric and asymmetric top), normal coordinates and their symmetry (CO_2), skeletal vibration and group frequency. Raman Effect, rotational and rotation- vibrational Raman transitions, nuclear spin effects, polarization of Raman lines.

Unit-3: Electronic Spectroscopy (10 L)

Absorption: L-B's Law and its limitations. Transition moment and its relation to molar extinction coefficient. Different types of transitions ($\pi\pi^*$, $\sigma\pi^*$, $n\pi^*$ etc.), Selection rules with symmetry arguments, Solvent perturbation method, Weak and CT transition, Vibronic and spin orbit coupling.
Emission: Basic principle and instrumentation, FC principle, Mirror-image symmetry and its violation, Radiative and radiationless deactivation, Polarization characteristics of emission, Fluorescence Quenching (static and Dynamics), Fluorescence lifetime measurement.

Reference books:

1. Cotton, F. A., *Chemical Applications of Group Theory.*
2. Mukherjee, A. K. and Ghosh, B. C., *Group theory in Chemistry.*
3. Banwell, C. N., Fundamentals of Molecular Spectroscopy
4. J. M. Hollas (Wiley, New York, 2004), Modern spectroscopy,
5. Donald A. McQuarrie and John D. Simon (Viva Books Private Limited, New Delhi, 1997) Physical Chemistry - A Molecular Approach;

Supramolecular Chemistry and its application (30 L) CHM21131

Introduction, Origins and Concept of Supramolecule. Molecular recognition. Host-guest complex. Supramolecular orbitals, non-covalent forces: soft interactions, Supramolecular reactivity and catalysis. Self-assembly and self-organisation, Liquid crystals and supramolecuar polymers, polymer-surfactant interaction. New molecular receptors: crown

ethers, siderophores, cyclophanes, cyclodextrin and their application in specific recognition processes. Supramolecular reactivity and catalysis, switching devices, self-assembly of supramolecular aggregates, crystal engineering.

Reference Books:

1. Lehn, J.-M. *Supramolecular Chemistry: Concepts and Perspectives.*
2. Das, A. K., *An Introduction to Supramolecular Chemistry.*

Analytical Chemistry Lab **CHM22095**

Course Content:

1. EDTA Titration of Ca^{2+} and Mg^{2+} in Natural Waters
2. Optimization of GC Analysis: the van Deemter Plot
3. Analysis of the Components in an Over-the-Counter Analgesic Drug using Ultraviolet Spectroscopy.
4. Determination of Iron in a Vitamin Tablet by Ultraviolet-Visible Spectroscopy
5. Error Propagation with Beer's Law
6. Use of pH meter: determination of pH of given dilute solutions of shampoos and soaps

Reference Books:

1. Daniel C Harris: Exploring Chemical Analysis.
2. Daniel C Harris: Quantitative Chemical Analysis.

Organic Chemistry Lab **CHM22096**

Course Content

1. Chromatography (Any one):
   a. Thin Layer Chromatography (TLC)
   b. Column chromatography **(**Separation of a mixture of two amino acids by ascending and horizontal paperchromatography, Separation of a mixture of two sugars by ascending paper chromatography, Separation of a mixture of o-and p-nitrophenol or o-and p-aminophenol bythin layer chromatography (TLC)
2. Representative reaction of esterification, ester hydrolysis, preparation of dyes, natural product extraction (caffeine, nicotine etc.) etc.

Reference Books:

1. Vogel's Text Book of Practical Organic Chemistry (5th Edition).
2. A Handbook of Organic Analysis: Qualitative and Quantitative (4th Edition) –Clarke.

Semester III

Spectroscopy and its application (45L) CHM21132

Unit I: Resonance Spectroscopy (NMR & ESR) (16 L)

Nuclear spin, nuclear resonance, saturation, relaxation, Basic instrumentation shielding and deshielding of magnetic nuclei, coupling constant, chemical shift and its measurements. Factors affecting chemical shift, spin - spin interactions and spin decoupling.

Principle of EPR and spin Hamiltonian (comparison to NMR spectroscopy), spectrometer, external standard, line-width, nuclear hyperfine interactions, anisotropy in Lande *g* factor and hyperfine interaction, magnetically equivalent and non-equivalent set of nuclei, intensity, structural information of organic radical and inorganic molecules from EPR spectra.

Unit-II: Fourier transformations (5 L)

Time domain versus frequency domain. Principles of FT NMR, instrumentation, the rotating frame of reference, simple 1D experiments. FT IR – principles and instrumentation

Unit III: Mössbauer spectroscopy (8 L)

Mössbauer activity: principle, experiment, line-width, centre shift, quadruple interaction, magnetic interaction; information of spin and oxidation states, structure and bonding, spin transition from spectra of different Mossbauer active nuclei in variety of environments.

Unit IV: Mass spectrometry (8 L)

Principles, instrumentation and applications of mass spectrometry. Methods of generation of ions in EI, CI, FD and FAB and other techniques. Detection of ions, ion analysis, ion abundance, molecular ion peak, metastable peak, isotopes, ion-molecule interaction and analysis of fragmentation patterns. Applications of mass spectroscopy to simple structural and mechanistic problems.

Unit 4: Photoelectron Spectroscopy (8 L)

Photoelectron spectroscopy: photoexcitation and photoionization, core level (XPS, ESCA) and valence level (UPS) photoelectron spectroscopy, XPS and UPS experiment, chemical shift, detection of atoms in molecules and differentiation of same element in different environments from XPS, information about the nature of molecular orbital from UPS, UPS of simple diatomic molecules, e. g., N_2, O_2, CO, HCl, etc.

Reference Books:

1. Sathyanarayana, D. N., *Handbook of Molecular Spectroscopy*
2. Das, A. K., Vol. 7. *Inorganic Chemistry*
3. Mossbauer Spectroscopy and Transition Metal Chemistry(Fundamentals and Applications)-Philipp Guetlich, Eckhardt bill, A. X. Trautwein
4. Electron Paramagnetic Resonance-Elementary Theory and Practical Applications-John A. Weil, James R. Bolton & John E. Wertz

Advance Physical Chemistry Special –I (45L) CHM21102

Unit-I: Advance Quantum Mechanics (10)

Spin: Stern-Gerlach expt. Spin and Pauli matrices. addition of angular momenta, Clebesch Gordan series, total angular momentum.

Hilbert space, Dirac notation, generalized uncertainty principle, position and momentum space representation. Continuous vs discrete basis, Delta function and Fourier transformation, Pictures- Schrodinger-Heisenberg-Dirac.

Unit-II: Approximation methods to solve quantum system (7)

1. Rayleigh-Schrodinger perturbation theory for non-degenerate states with simple applications. Degenerate perturbation theory-Stark effect. First and second order lifting of degeneracy.
2. Variation method: Basis and applicability. Linear variation method- secular determinant.

Unit-III: Theoretical aspects of spectroscopy (13)

Time dependent perturbation theory: semi classical treatment of interaction of matter with radiation, first and second order effects, Fermi golden rule, selection rule, selection rule for vibrational spectra, anharmonicity correction by perturbation – appearance of overtones; selection rule for rotational spectra, nuclear spin and rotational energy levels. Selection rule for rotational and vibrational Raman spectroscopy; Quantum mechanical theory of magnetic resonance; Bloch equations and their solutions; theories of shielding – diamagnetic and paramagnetic shielding

Unit IV: Group theory and application (15)

Abstract Group theory revisited. Construction of direct product group, C_5 and C_6 point group. MO theory with applications to σ and σ* bonding and construction of hybrid orbitals. Hückel theory MO construction for naphthalene, pyridine etc. Symmetry and chemical reactions; Woodward –Hoffmann Rule: Diel Alder reaction: dimerization of ethylene and Diels-Alder reaction. Application of group theory to Ligand and crystal field theory.

References:

1. Quantum Chemistry, I.N. Levine, Pearson Educ., Inc. New Delhi.
1. 2.Introduction to Quantum Mechanics. D. J. Griffiths, Prentice Hall.
2. Molecular Spectroscopy, I. N. Levine, Wiely-Interscience Publication.
3. Molecular Spectroscopy, J. L. McHale, Taylor & Francis.
4. Quantum Mechanics, B. H. Bransden and C. J. Joachen. Pearson.
5. Chemical Application of Group Theory, F. A. Cotton, Wiely Student edition.

Advance Physical Special II (45L) **CHM21103**

Unit I: Advanced Electrochemistry: **(20L)**

Limitation of Debye-Hückel limiting law and its extension; Pitzer ion-interaction approach.Debye-Hückel-Onsagar (DHO) theory of electrical conduction of electrolytes, electrophoretic and relaxation effects, Wien effect, Debye-Falkenhagen effect, application of DHO theory.Limitation of DHO equation and Shedlovsky approach. Double layer studies: nature of the double layer across electrode-solution interface, polarizable and non-polarizable electrodes, electrocapilarity (EC) – nature of EC curves, its thermodynamics, Lipmann equation, Helmholtz, Guoy-Chapman and Stern double layer models. Electron transfer reactions; fuel cells.

Unit II: Polymer Chemistry **(13L)**

1. Introduction: Classification of polymers, intermolecular forces in polymers.
2. Mechanism and kinetics of step-growth and chain growth polymerization: Radical, cationic, anionic and condensation polymerization, copolymerization, reactivity ratios, thermodynamic aspects of polymerization
3. Polymer solutions: Flory-Huggins theory of polymer solutions, nature, size and shape of macromolecules in solution.
4. Polymer structure and Physical properties: Microstructure of polymer chains, crystallinity in polymers, glass transition temperature, rheological properties, molecular weight and its distribution.
5. Specialty polymers: Liquid crystalline polymers, conducting polymers, electroluminescent polymers, inorganic polymer, nanocomposites of polymers, biomedical polymers.

Unit III: Surface Chemistry and catalysis **(12 L)**

Bimolecular surface reactions: reaction between a gas molecule and an adsorbed molecule, Langmuir isotherm, BET isotherm (with derivation), inhibition and activation energy of surface reactions, catalytic activity at surfaces (volcano curve), unimolecular and bimolecular surface reactions, comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity.

References:

1. Text Book of Polymer Science, F.W. Billmayer Jr., 3rd Edition (1984), Wiley-Inter
1. Science, New York
2. E.M. Mc Cash, Surface Chemistry, Oxford University Press, Oxford (2001).
3. Physical Chemistry, P. W. Atkins, 8th Ed., Oxford University Press, New York
4. Modern Electrochemistry, Vol. 2 A & B, J.O'M. Bockris and A. K. N. Reddy, 2nd Ed.
5. Plenum Press, New York
6. An Introduction to electrochemistry, S. Glasstone

Or

Advanced Inorganic Special I (45L) CHM21104

Unit-I: Organometallic Chemistry (15 L)

Reaction of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands. Inorganic π-Acid Ligands: Dioxygen and dinitrogen, nitrosyl, tertiary phosphines and arsines as ligands. Complexes of σ-donor ligands: Transition metal alkenyls, alkynyls, carbenes and carbynes. π-complexes of unsaturated molecules: Preparation, bonding and structure of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis. Fluxionality in organometallic complexes.

Transition metal Compounds with M-H bonds: Metal hydrides (classical and nonclassical). Agostic interaction. Application of NMR in studying hydrido complexes.
Application of organometallic chemistry: alkene metathesis, dimerization, oligomerization and polymerization of alkenes, activation of CO, CO_2, CH activation.

Unit-II: Borane Chemistry (15 L)

Metallaboranes, Metallacarboranes, metal σ and μ bonded borane/carborane clusters. Resemblance of Metallaboranes/ Metallacarboranes with ferrocene and related compounds.Applications of Metallaboranes/Metallacarboranes as drug delivery system.Applications of PSEPT over heteroboranes. Principle of Isolobility: Development and formulation of the concept of isolobility and its applications in the understanding of structure and bonding of heteroboranes.

Unit-III: Inorganic rings and clusters (15 L)

Metal-metal bonding (MO approach), metal-metal single and multiple bonded compounds. Bonding in dimolybdenum and dirhenium complexes. Application of isolobal and isoelectronic relationships. Synthesis, structure, reactions and bonding as applicable in respect of molybdenum blue, tungsten blue, ruthenium blue, platinum blue, tungsten bronze, ruthenium red. Iso-and hetero-polyoxometalates of V, Mo and W: synthesis, structure, reactions and uses. Low nuclearity (M_3, M_4) and high nuclearity (M_5-M_{10}) carbonyl clusters: skeletal electron counting.

Reference Books:

1. Cotton, F.A. & Wilkinson, G. *Advanced Inorganic Chemistry*, Wiley, VCH, 1999.
2. Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. *Concepts & Models of Inorganic Chemistry*
3. B. D. Gupta and A. J . Elias, *Organometallic Chemistry*
4. Cotton, F.A. & Wilkinson, G. *Advanced Inorganic Chemistry*

Advanced Inorganic Special II (45L) CHM21105

Unit – I: Magnetochemistry (30 L)

Definition of magnetic properties, types of magnetic bodies, experimental determination of magnetic susceptibility: Gouy method, VSM, SQUID. Anisotropy in magnetic susceptibility.

Diamagnetism in atoms and polyatomic systems. Pascal's constants, two sources of paramagnetism, spin and orbital effects, spin-orbit coupling, Lande interval rule, energies of J levels, Curie equation, Curie's law, Curie-Weise law, van Vleck equation and its application, first order and second order Zeeman effects, temperature independent paramagnetism, magnetic properties of transition metal complexes in cubic and axially symmetric crystal fields, low spin-high spin cross-over, photo magnetism, spintronics, single ion magnet, single molecular magnetic, single chain magnet, magnetic behavious of lanthanides and actinides, magnetic exchange interactions.

Unit – II: Solid state chemistry-I (15 L)

Defects in solids, point, line and plane defects, determination of equilibrium concentration of Schottky and Frenkel defects, stoichiometric imbalance in crystals and non-stoichiometric phases, colour centres in ionic crystals, band theory, band gap, metals, insulators, semiconductors (intrinsic and extrinsic), hopping semiconductors, rectifiers and transistors, bonding in metal crystals, free electron theory, electronic specific heat, Hall effect, electrical and thermal conductivity of metals, superconductivity, Meissner effect, basic concept of BCS (Bardeen-Cooper-Schriffer) theory.

Reference Books:

1. Earnshaw, A., *Introduction to Magnetochemistry*
2. Dutta and Shyamal, *Elements of Magnetochemistry*
3. Das, A. K., Vol. 6, *Inorganic Chemistry*
4. West, A. R., *Solid State Chemistry and its Applications*

Or

Advance Organic Special –I (45L) CHM21106

Unit I: Stereochemistry (15L)

Diastereoselective synthesis: Asymmetric synthesis with chiral substrates (Cram's rule, Felkin Anh model, Prelog's rule, Stereochemistry of reactions– nucleophilic additions to cyclic ketones, Cieplak model.

Chiroptical properties of organic molecules, CD, ORD-principles and applications, haloketone rules, sector rules.

Chiral analysis by Polarimeter, NMR, GC, HPLC and 29 Capillary Electrophoresis (CE) methods, hydrolytic kinetic resolution.

Unit II: Organic Photochemistry and Radical Reactions (30L)

Photochemistry: Photolysis of carbonyl compounds and nitrites: Norrish Type I and Type II processes, α-cleavage, Barton reaction. Photoreduction and Photoexcitation; Photorearrangements in cyclohexanones and cyclohexadienone systems; Photorearrangements of α-tropolone methyl ether, di-π-methane rearrangement (cyclic system) Photochemistry of organic compounds: photoisomerisation, phodimerisation, cycloadditions of benzene and its derivatives.

Radical Chemistry: Generation and detection of radicals, radical initiators, reactivity pattern of radicals, substitution, addition and cyclization reactions; Radical cations and radical anions, single electron transfer reactions.

Reference Books:

1. Stereochemistry of Organic Compounds - E. L. Eliel and S. H. Wilen.
2. Stereochemistry of Organic Compounds - D. Nasipuri.
3. Organic Photochemistry - J. W. Coxon& B. Halton.
4. Elements of Organic Photochemistry - D. O. Cowan & K. L. Drisco.
5. Radical Chemistry: The Fundamentals-M.J. Perkins (Oxford Chemistry Primers)

Advance Organic Special –II (45L) CHM21107

Unit I: Medicinal Chemistry-I (20L)

An overview of drugs and drug targets at the molecular level; intermolecular binding forces. Classification of drugs. Pharmacodynamic (PD) studies: Enzymes as drug targets, Receptors as drug targets, Nucleic acid as drug targets, Miscellaneous drug targets (biosynthetic building blocks, transport proteins etc as drug targets). Pharmacokinetics (PK) studies: Drug ADME, Drug administration, Drug dosing, Drug delivery. Prodrugs and use of prodrug systems (prodrugs for stability, solubility and slow release), overview of drug delivery; Synthetic methods in medicinal chemistry: Combinatorial and parallel synthesis: solid phase techniques, mix and split method in combinatorial synthesis; dynamic combinatorial synthesis; solid phase synthesis; diversity-oriented synthesis. Lead discovery; Bioassays; drug targets; Lead Modification; optimization; pharmacophore. Quantiative-structure activity relationships (QSAR). Toxicological studies for drugs: Therapeutic index and therapeutic window, ED-values, LD-values. drug synergy.

Unit-II: NMR Spectroscopy (10L)

Principle, instrumentation and different techniques (CW & FT) of NMR spectroscopy, classification of A4, A3, ABX, AMX, ABC, A2B2 in proton NMR. Introduction to ^{13}C-NMR spectroscopy, DEPT, application of NMR spectroscopy and other spectroscopical techniques to simple structural and mechanistic problems.

Unit III: 2D NMR-Application in Organic Chemistry (15L)

Application of ^{1}H-^{1}H COSY, ^{1}H-^{13}C HETCOR, HMBC, HMQC, HSQC, TOCSY, NOESY in structure elucidation of organic compounds, reaction monitoring etc., Solid state NMR, Chemical Shift Anisotropy and Cross Polarisation, MRI as a diagonistic tool. Solving structural problems using 2D NMR.

Reference Books:

1. Biochemistry by Voet and Voet.
2. Organic Chemistry of Drug Design and Drug Action (3rd Edition)- R. Silverman
3. Introduction to Medicinal Chemistry (6th Edition)- G. L. Patrick.

4. Spectrometric Identification of Organic Compounds – R. M. Silverstein & F. O. Webster; 6th edition
5. Applications of Nuclear magnetic Resonance Spectroscopy in Organic Chemistry L. M. Jackman.
6. Introduction to Spectroscopy (5^{th} Edition) - D.L. Pavia
7. NMR and Chemistry – J. W. Akitt. Organic Spectroscopy – W. Kemp, 3rd Edn.

Advanced Special Practical-1 **CHM22108**

Physical Chemistry:

Programming

Application of FORTRAN in scientific computing

- To prove uncertainty principle for particle in 1D box, SHO
- Lifting of degeneracy.
- Construction of Huckel MO
- Energy minimization on Potential energy surface
- Gillespie Algorithm

software based experiments

- Molecular modelling
- Gaussian16

Reference:

1. Fortran77 and Numerical Methods, C Xavier, New Age International (P) Ltd.
2. Modern Fortran in Practice, Arjen Markus, Cambridge Univrsity Press (2012).
3. Numerical Recipe in Fortran77, The art of scientific computing. W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, 2^{nd} Edition, Cambridge Univrsity Press.
4. Quantum Chemistry, I.N. Levine, Pearson Educ., Inc. New Delhi.
5. .Introduction to Quantum Mechanics. D. J. Griffiths, Prentice Hall.
6. Gillespie D T 1976 *J. Comp. Phys.* **22** 403
7. 2. Gillespie D T 1977 *J. Phys. Chem.* **81** 2340
8. An introduction to Genetic Algorithm, Melanie Mitchell, The MIT Press
9. Kirkpatrick K S, Gelatt C D and Vecchi M P 1983 *Science* **220** 671.

Inorganic Chemistry Practical:

- Estimation of Cr in steel
- Estimation of Ti in bauxite sample
- Estimation of Zn in brass sample

- Estimation of iodine in salt
- Estimation of Fe_2O_3 in cement

Organic Chemistry Practical

Course Content

1. Synthesis, purification and Identification of bioactive/drug molecules (Paracetamol**,** Phenytoin, methyl red, Hippuric acid etc.)
2. Quantitative analysis of (i) sulphur and (ii) nitrogen.

Reference Books:

1. Khosla, B. D.; Garg, V. C. & Gulati, A., Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).

Halpern, A. M. &McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

Project and Dissertation-1 **CHM25109**

Course Content:

Chemistry is the science of matter, especially its properties, structure, composition, behavior, reactions, interactions and the changes it undergoes. Chemistry is sometimes called 'the central science' because it connects physics with other natural sciences such as astronomy, geology and biology. On completion of 5th Semester of B.Sc. Chemistry students will be acquainted with advance knowledge in Chemistry both theoretically and practically. Students are supposed to choose a research project allied to their expertise and chemical sciences. Students are expected to carry on the chosen research project and note down observations to reach out a possible scientific inference regarding the chosen project. On the completion of project work, students should submit their 'dissertation'.

Corrosion and Corrosion control system (30L) **CHM21110**

Course Content:

Unit I: Electrochemistry of corrosion

Corrosion – introduction, definitions and types; Electrochemical cells-definitions and principles; Potential measurements - galvanic cells, concentration cells; EMF and Galvanic series - bimetallic couples; Eh-pH diagrams – fundamental aspects; Construction of Eh – pH diagrams. FeH_2O-O_2 diagram; Copper, Aluminium and general corrosion diagrams.

Unit II: Electrode kinetics and polarization phenomena

Electrode – solution interface – definition and types of polarization; Exchange current density ; polarization relationships; Polarization techniques – corrosion rate determination; Mixed

potentials – concepts and Basics. Mixed potential theory – bimetallic couples; Mixed potential theory

Unit III: Prevention strategies

Design and coatings; Prevention strategies – inhibitors and surface engineering. ; Cathodic protection; principles and classification; Cathodic protection – influencing factors and monitoring; Design aspects for cathodic protection; Stray current corrosion.;Passivity – definitions and influencing parameters

Unit IV: Biological aspects of corrosion

Microbially influenced corrosion (MIC) – definitions, environments and microbiology; Electrochemical aspects and general mechanisms; Bacterial transport, attachment and affected materials

Reference Books:

1. Modern Electrochemistry, J.O'M. Bockris and A. K. N. Reddy, Vol. 2 A & B, 2nd Edition,
2. Plenum Press, New York (1998).
3. Electrochemical Methods: Fundamentals and Applications; A.J. Bard and L.R. Faulkner, 2nd

Or

Strategies in Organic Synthesis (30L) CHM21111

Course Content

Unit-I: Organoboron (6L)

Chemistry of organoboron compounds, carboranes, hydroboration, reactions of organoboranes, unsaturated hydrocarbon synthesis, allylboranes, boronenolates.

Unit-II: Organophosphorus (6L)

Chemistry of organophosphorus compounds, Phosphorus ylides and chiral phosphines.

Unit-III: Organosilicon compounds (6L)

Chemistry of organosilicon compounds, Synthetic uses of silyl ethers, silylenol ethers, TMSCN, alkene synthesis, alkynyl, vinyl, aryl, allyl and acyl silanes; Brook rearrangement, silicon Baeyer Villiger rearrangement

Unit-IV: Organosulphur (6L)

Chemistry of organosulphur compounds, Sulphur- stabilized anions and cations, sulphonium salts, sulphonium and sulphoxoniumylides, chiral sulphoxides, umpolung Nitrogen ylide, oxoniumylide

Unit-V: C-H Functionalization in organic synthesis (6L)

Mechanisms of C-H bond activation with transition metals, Organic synthesis involving chelationassisted C-H activation, ortho-C-H activation, C-H activation in heterocycles and base-assisted C-H activation. C-H, C=C and C≡C activated annulation reactions. Important synthetic approaches via C-X (X= C, N, O, S etc.) bond activation. Role of non-metallic activation of bonds in organic synthesis.

Reference Books:

1. Hydroboration - H. C. Brown
2. Borane Reagents - H. C. Brown, A. Pelter, K. Smith.
3. Relevant parts from Advanced Organic Chemistry - F.A. Carey and R.J. Sandberg; Vols. I & II.
4. Relevant parts from Comprehensive Organic Synthesis - B. M.Trost& I. Fleming
5. Principles of Organic Synthesis - RO.C. Norman and J. M. Coxon-Blackie.
6. C-H Bond Activation in Organic Synthesis - Jie. J. Lee

Or

Bio-inorganic Chemistry (30L) **CHM21112**

Dioxygen storage/transport proteins: haemoglobin, myoglobin, hemerythrin and hemocyanin. Di-nitrogen fixation. Electron transport proteins: cytochromes, Fe-S proteins and other electron carrier proteins in biology. Metalloproteins catalysing oxygen atom transfer reaction: iron containing enzymes such as methane monoxygenase, nitric oxide reductase; Molybdenum containing enzymes such as xanthane, sulphite oxidase and nitrate, trimethylamine-N-oxide, DMSO reductase. Other selected metalloproteins of various metal ions. Structure/function analogue of above mentioned systems. respiratory electron transport chain and photosynthetic electron transport chain, Toxic metal ions and their effects, chelation therapy, Pt and Au complexes as drugs, metal dependent diseases.

References:

1. S.J. Lippard & J.M. Berg, *Principles of Bioinorganic Chemistry*
2. G. N. Mukherjee and A Das, *Bioinorganic Chemistry*
3. Asim K Das, *Bioinorganic Chemistry*

Or

Any Suitable UGC-MOOCs Course **CHM21113**
Internship in Industries **CHM24114**

Semester IV

Contemporary research methodologies and data analysis CHM22130

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus, WoS, CCDC and ICSD.

Methods of Scientific Research and Writing Scientific Papers:

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation. Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism. Training on instrumental data collection and conversion, data analysis and data interpretation. Training on several scientific software (like ChemDraw, Origin, Apex, Wingx, Mercury, Diamond 3.1, MNova, Xshell, TOPOS, SHAPE 2, Gaussian etc.)

Chemical Safety and Ethical Handling of Chemicals:

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals.

Materials Science and Nanotechnology (30L) CHM21115

Course Content

Unit-I: Nanomaterials: Inorganic and Biomaterials (15 L)

1. Different synthetic routes: Physical, Chemical, Mechanical and electrochemical methods of nanomaterial design, Control of growth kinetics/seeding kinetics, morphology and structure, Classifications of nanosystems: 0D, 1D, 2D, 3D Nanomaterials, Size dependent properties of nanomaterials - Quantum Confinement Effects, Electronic properties and their optical behavior changes, Surface Plasmon Resonance (SPR), Direct and Indirect Transitions: Discussions on Nanoclusters and Nanowires; Metal, Metal Oxide, semiconductor nanoparticles, Carbon Nanotubes, 2-D Nanopatterns and Self-assembled Monolayers on Inorganic Substrates; Mesostructured and Mesoporous Materials; Inorganic-Organic and Inorganic-Polymer Nanocomposite Materials; Protein based nanostructures Hybrid organic-inorganic nanomaterials (functionalized nanomaterials) and its wide application towards different sensor, SAMS (self-assembly of monolayers) films, Core-shell nanosystems. Differences between Light Microscope (LM) and Electron Microscope (EM), X-ray diffraction, SEM-EDX, TEM/HRTEM, DLS and electrical/thermal conductivity of nanomaterials.

Unit-II: Applications of Nanotechnology: Electronics, Chemical and in Biomedical Fields (15 L)

Advantages of nano electrical and electronic devices, , Lighting and Displays, Batteries - Fuel cells and Photo-voltaic cells, nanoparticle coatings for electrical products. Nanocatalyts, Smart materials, Heterogenous nanostructures and composites, Nanostructures for Molecular recognition (Quantum dots, Nanorods, Nanotubes), Molecular Encapsulation and its applications, Nanoporous zeolites, Self-assembled Nanoreactors, Electrospinning – Controlling morphologies of nanofibers, , Cosmetics, Formulation of Gels, Shampoos, Hair-conditioners, Sun-screen dispersions for UV protection using Titanium oxide, color cosmetics. Inorganic (metal/metal-oxide) nanoparticles and nucleic acid and protein based recognition groups, Application in optical detection methods, Nanoparticles in bone substitutes and dentistry, Photodynamic Therapy, Nanobiosensors in Diagnosis, Inorganic metal oxide/lanthanides as MRI agents, Drug delivery, Artificial life, Hybrid materials, Future of Bionanotechnology. Fertilizer and pesticides. Nanotechnology in Food industry.

Reference Books:

1. C. N. R. Rao, A. Muller, A. K. Cheetham, *The Chemistry of Nanomaterials: Synthesis, Properties and Applications,* Volume 1, Wiley-VCH, Verlag GmbH, Germany (2004).
2. C. Brechignac P. Houdy M. Lahmani, *Nanomaterials and Nanochemistry***,** Springer Berlin Heidelberg, Germany (2006).
3. Guozhong Cao, *Nanostructures &Nanomaterials Synthesis, Properties G;Z: Applications*, World Scientific Publishing Private, Ltd., Singapore (2004).
4. Carl C. Koch, *Nanostructured Materials: Processing, Properties and Potential Applications, N*oyes Publications, William Andrew Publishing Norwich, New York, U.S.A (2002).
5. C. M. Niemeyer, C. A. Mirkin-*Nanobiotechnology: Concepts, Applications and Perspectives*‖, Wiley – VCH, (2004).

6. T. Pradeep, ―*Nano: The Essentials*‖, McGraw – Hill education, (2007).

Or

Natural Products and Bio-Organic Chemistry (30L) CHM21116

Unit-I: Natural Products (15L)

Familiarity with methods of structure elucidation (chemical &spectroscopical method), biosynthesis, synthesis and biological activity of alkaloids (nicotine, atropine, coniine and papaverine), terpenoids and steroids (representative examples). Total synthesis of few of the natural products from the following list: Strychnine (Woodward), Strychnine (Overman), Penicillin V (Sheehan), Reserpine (Woodward), Vitamin B12 (Woodward), Progesterone (Johnson), Prostaglandins F2-alpha and E2 (Corey), Prostaglandins A2 and F2-alpha (Stork), Carpanone (Chapman), Monensin (Kishi), Monensin (Still), Biotin (Baggiolini), Periplanone B (Still) *etc*.

Unit-II: Bio-organic Chemistry (15L)

Enzyme catalyzed reactions – examples of nucleophilic displacement on a phosphorus atom, enzymatic action of some common enzymes like chymotrypsin, lysozyme, ribonuclease, carboxypeptidase etc; coupling of ATP cleavage to endergonic processes, proton transfer reactions to and from carbon. Chemistry of coagulation; Chemistry of vision; Chemistry of electron transport; Chemistry of decarboxylation; Chemistry of biological methylation. Use of enzymes in organic synthesis (biocatalysis); Biotechnological applications of enzymes: Enzyme purification, immobilization of enzymes, enzyme therapy, enzyme and recombinant DNA technology. Molecular models of biological receptors, biomimetic chemistry, design, synthesis and binding studies of synthetic receptors. Enzyme models, micelles, polymers, cyclodextrins, remote functionalization reactions, catalytic antibodies, principle of gene synthesis.

Reference Books:

1. Natural Product Biosynthesis: Chemical Logic and Enzymatic Machinery- Christopher T. Walsh
2. The Organic Chemistry of Biological Pathways (2nd Edition)- John E. McMurry; Tadhg P. Begley
3. Bioorganic Chemistry- Dugas
4. Classics in Total Synthesis: Targets, Strategies, Methods (1st Edition)-Nicolaou, Sorensen.

Or

Any Suitable UGC-MOOCs Course CHM21117

Advance Physical Special –III (45L) CHM21121

Unit-I: Modern Spectroscopy (13)

1. Lasers: Einstein's two level transition model, Principles of laser action, two level system, three level system, laser characteristics, pulsed lasers, laser cavity modes, Q-switching, mode locking, non-linear effects, harmonic generation, examples of lasers: He-Ne, Nd-YAG, titanium-sapphire., dye lasers.
2. Single molecule spectroscopy: Fluorescence microscopy, single molecule detection, confocal detection optics and configuration, applications.
3. Lasers Raman spectroscopy: Stimulated Raman spectroscopy (SRS), surface enhanced Raman scattering (SERS), hyper-Raman, Coherent anti-Stokes Raman spectroscopy (CARS).

Unit-II: Magnetic resonance (12)

A review of spin angular momentum, basic principles and relaxation times, intensity of NMR signals, electronic shielding, NMR in liquids: chemical shifts, spin-spin couplings, NMR spectra of AX, A3X and AB systems. ESR of hydrogen, first order hyperfine energies, ESR of organic radicals in solution. FT-NMR: Rotating frame of reference, effect of RF pulses, FID, Multipulse operation, measurement of T1 by inversion recovery method, spin echo and measurement of T2, 2-D NMR, NMR hardware.

Unit III: Principles of Photochemistry (10)

Introduction to Molecular Photochemistry; Absorption; Electronic transitions: Frank-Condon principle, selection rules; photodissociation, predissociation, photoreduction, photooxidation, photodimerization; Advanced photochemistry techniques; Photochemical Reactions; Photochemical Reaction Mechanisms; Photoredox Catalysis. Electronic Excited States; Deactivation of Excited States; Energy and Electron Transfer; Life time of electronically excited state, fluorescence quenching, Stern-Volmer relation.

Unit IV: Biophysical Chemistry (10)

Structure, conformation, interactions and folding of biological macromolecules; methods of determination of structures of macromolecules (XRD, neuron diffraction, scattering from solutions of macromolecules); thermodynamic principles/titration and scanning calorimetry; sedimentation, electrophoresis; mass spectrometry, uv/vis absorption, Spectroscopic methods: steady state and time resolved techniques, fluorescence quenching, anisotropy and FRET as a tool of protein-protein or protein-drug interactions, circular dichroism; osmotic stress/molecular crowding; equilibrium dialysis single molecule technique, Separation techniques : Gel Electrophoresis. Macromolecule-ligand binding and cooperativity.

References

1. Applications of Nuclear magnetic Resonance Spectroscopy in Organic Chemistry L. M. Jackman.
2. NMR and Chemistry – J. W. Akitt.

3. Modern Spectroscopy – J.M. Hollas
4. Laser Spectroscopy – W. Demtroder
5. Principles of Physical Biochemistry – K.V. van Holde, C. Johnson, P.S. Ho
6. Physical Chemistry of Macromolecules – C. Tanford
7. Organic Photochemistry - J. W. Coxon& B. Halton
8. Single Molecule Spectroscopy, R. Rigler, M. Orrit, T. Basche
9. Handbook of Single Molecule Fluorescence Spectroscopy, C Gell, D. Brockwell, A. Smith
10. Principles of Fluorescence Spectroscopy, J. Lakowicz

Advance Physical Special IV (45L) **CHM21122**

Unit-I: Quantum Chemistry **(15)**

1. Born-Oppenheimer (B.O.) approximation. Many-electron systems: Closed and open shells, Antisymmetric principle and antisymmetrizer operator. Independent particle model (IPM). Self-consistent fields. Hartee and Hartee-Fock(HF) Theories. HF methods for closed shells. Implementation of HF method for closed shells: Roothan equation. HF theory and Koopmans' theorem. Problems with open-shell systems. Restricted and unrestricted HF methods.
2. Electron correlation. Multideterminantal wave function and CI. Brillouin's theorem.
3. Rudiments of Density Functional Theory: Expectation Value calculation using density: Kohn-Hohnenberg Theorems; Kohn-Sham equation for the ground state of many body systems.

Unit-II: Statistical Mechanics **(15)**

1. Phase space, ergodic hypothesis, Liouville's theorem, Concepts of different ensembles with applications to selective systems. Fluctuations. Prefect gas, System of interacting molecules, treatment of imperfect gases.
2. Quantum Statistics: Classical limits of Fermi-Dirac and Bose-Einstein distribution; Application of the quantum statistics for deriving thermodynamic properties of ideal BE and FD systems (conduction electron, black-body radiation, Bose Einstein condensation), density matrix

Unit-III: Solid state chemistry-II **(15)**

1. Fourier synthesis of a crystal structure: Diffraction of waves by crystals; Fourier analysis; Reciprocal lattice vectors; Diffraction condition; Laue equations; Ewald construction; Brillouin zone; Reciprocal lattice to cubic lattices; Fourier analysis of the basis; Structure factor; Systematic absences; Atomic scattering factor.
2. Free electron theory of metals: Free electron gas in 1D and 3D; Fermi-Dirac distribution function; Fermi surface; Electron velocity at the Fermi surface; Density of states; Heat capacity; Electrical conductivity; Matthiessen's rule; Thermal conductivity; Wiedemann-Franz law; Hall Effect.

3. Junction Properties: Metal-metal, metal-semiconductor and semiconductor-semiconductor junctions; p-n junction; Photovoltaic effect and solar cells.

References:

1. Quantum Chemistry, I.N. Levine, Pearson Educ., Inc. New Delhi.
2. Quantum Mechanics, B. H. Bransden and C. J. Joachen. Pearson.
3. Modern Quantum Chemistry, A. Szabo and N. S. Ostlund, Dover Publication, New York.
4. Density-Functional Theory of Atoms and Molecules; Robert G. Parr, Weitao Yang, Oxford University Press.
5. Statistical Mechanics, D. A. McQuarrie, Harper & Row
6. Introduction to Solid State Physics, C. Kittle. Wiley India.
7. Statistical Mechanics, R.K.Pathria, P.D.Beale, Elsevior.
8. Elementary solid state physics, M.A. Omar, Pearson

Or

Advance Inorganic Special III (45L) CHM21123

Unit-I: Spectroscopic Application in Inorganic Systems (15 L)

Plane polarized light, CD, ORD and MCD spectra. Experimental aspects of absolute configuration of coordination compounds. Advanced EPR spectroscopy and Mossbauer spectroscopy and their applications in inorganic and bio-inorganic chemistry. NMR spectra: ^{11}B, ^{13}C, ^{19}F, ^{27}Al, ^{31}P NMR spectroscopy with typical examples, ^{1}H-NMR spectra of coordination compounds of paramagnetic metal ions, dipolar and contact shifts, magnetic susceptibility and resonance shift. NQR spectroscopy: Principle, nuclear quadrupole coupling constant, structural information from NQR spectra.

Unit-II: Chemical Applications of Group Theory (15 L)

(i) IR and Raman Spectroscopy: Brief introduction to molecular vibrations; selection rules for fundamental vibrational transitions, symmetry of normal modes of molecules, Infrared and Raman activity of some typical molecules (molecules of C_{2v}, C_{3v}, C_{4v}, D_{2h}, D_{3h}, D_{4h}, T_d and O_h point groups)

(ii) Crystal Field Theory: Splitting of levels and terms in chemical environment, construction of energy level diagrams, selection rules and polarizations.

(iii) Molecular Orbital Theory: Introduction, transformation properties of atomic orbitals; hybridization schemes for s- and p-bonding, hybrid orbitals as LCAOs; Molecular Orbital Theory for some typical AB_n types (n = 2, 3, 4, 6) of molecules (H_2O, NH_3 and BH_3)

(iv) Electronic Spectra: General considerations, typical examples from tetrahedral and octahedral systems, Orgel energy level diagrams.

Unit-III: Nuclear Chemistry and Radiochemical Analysis (15 L)

Nuclear models – Nuclear forces, liquid drop model, Fermi gas model, Shell model. Magic numbers. Nuclear spin and nuclear isomerism. Radiation dosimetry. Artificial Nuclear Reactions: Various important nuclear reactions, Nuclear reactions versus chemical reactions, Classification of nuclear reactions. Nuclear Fission: Spontaneous fission, Mechanism of nuclear fission, Chain reactions of fissions, Atom bomb, Nuclear reactor, Radiolysis of water.

Application of radioactivity in geochemistry and cosmochemistry, methods of age determination, radioactive analysis. Tracer techniques: study of chemical reactions, isotopic exchange reactions, kinetic isotope effect.

Reference Books:

1. Das, A. K., Vol. 7, *Inorganic Chemistry*
2. Cotton, F. A., *Chemical Applications of Group Theory*
3. Mukherjee, A. K. and Ghosh, B. C., *Group theory in Chemistry*
4. Arnikar, H. J., *Nuclear Chemistry*

Advance Inorganic Special IV (45L) CHM21124

Unit-I: Inorganic Reaction Mechanism (15 L)

Mechanism of substitution reactions: Solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation, pseudo-substitution. Four broad classes of mechanism of substitution – D, A, I_a and I_d mechanism of isomerisation reaction–linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racemisation, Ray–Dutta and Bailar twist mechanisms. Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, self-exchange reactions. Outer sphere and inner sphere reactions, applications of Marcus expression (simple form), redox catalysed substitution reactions.

Unit-II: X-ray Crystallography (20 L)

Crystal and lattice, process of crystallizations, crystal form, habit, defect, lattice planes, indices, crystal systems and symmetry, primitive and non-primitive lattice, diffraction of X-ray, Brag's condition, reciprocal lattice, Brag's law in reciprocal lattice, Ewald sphere, X-ray Crystallography Instrumentation, goniometer, geometric data collection, lunes, crystal mosaicity and beam divergence, completeness of data collection, crystal to detector distance vs resolution, atomic scattering factor, structure factor, intensity of diffracted beam, Friedel's Law, systematic absences, temperature factor on the intensity of diffracted beam.

Unit-III: Photo inorganic chemistry (10 L)

Photochemistry of Transition Metal Complexes: Photoreactions of complexes of Cr(III) and Co(III), photo-aquation, photo-substitution and photo-racemization Photochemistry of $Ru(bpy)_3^{2+}$and its application as photocatalyst for photo-splitting of water, photooxidation of 2-propanol and photo-reduction of carbon dioxide, cyanide bridged triruthenium(II) bipy complexes as antenna. Photochemistry of diisocyanide bridged dimers of Rh(I). Applications

of quenching and sensitization techniques in the identification of reactive state in coordination complexes.

Reference Books:

1. F. Basolo and R.C. Pearson, *Mechanisms of Inorganic Chemistry*
2. West, A. R., *Solid State Chemistry and its Applications*
3. Hebbar, K. R., Basics of X-Ray Diffraction and its Applications
4. Rohatgi-Mukherjee, K. K., *Fundamentals of Photochemistry*
5. Hammer, F., *Inorganic Photochemistry*

Or

Advance Organic Special-III (45L) CHM21125

Unit-I: Asymmetric Synthesis (20L)

Principles; Addition to carbonyl compounds: use of chiral substrate, chiral reagent, chiral catalyst; stereoselective formation of E/Z-alkene, Stereoselective reactions of carbonyl compounds: enolate formation, alkylation, asymmetric aldol reactions; Stereoselective reactions of alkenes: Diels-Alder reaction, sigmatropic rearrangement, stereoseletive hydrogenation, epoxidation, hydroxylation, aminohydroxylation, cyclopropanation; Kinetic resolution; Asymmetric synthesis of menthol (Takasago), crixivan (Merck)Enantio- and diastereoselective synthesis, Biotine synthesis, LFT synthesis, Gerner's aldehyde synthesis. Stereoselective Rearrangement: [3,3]-Sigmatropic, (2,3)-Wittig, alkene isomerisation. Introduction to organo-catalysts and its application.

Unit-II: Application of Translational Metal and Modern Reagents in Organic Synthesis (20L)

Application of organotransition metals in organic synthesis-preparative, structural and mechanistic aspects (with special thrust on Pd). Davies rule, catalytic nucleophilic addition and substitution reaction, Coupling reaction:Heck, Sonogashira, Kumada, Negeshi, Stille, Suzuki coupling Ziegler Naata reaction, Olefin metathesis, Tebbe's reagent, Pauson-Khand reactions, Volhardt co-trimerisation, functional organometallic compounds. Use of nontransition metal Indium, tin, zinc. Use of the following reagents: Complex metal hydrides, Gilman's reagent, lithium dimethylcuprate, lithium diisopropylamide (LDA), dicyclohexylcarbodiimide, 1,3-dithiane (reactivity Umpoloung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and pervost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, Phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast.

Unit-III: C-H bond activation (5L)

Introduction of C-H bond activation, Transition metal catalysis, Mechanisms of C-H bond activation with transition metals (Oxidative addition, sigma bond metathesis, electrophilic and metallo radical activation). Organic synthesis involving chelation-assisted C-H activation, ortho-C-H activation, meta-C-H activation (basic idea), para-C-H activation (basic idea) in carbocycles/heterocycles.

Reference Books:

1. Principles of Organic Synthesis - RO.C. Norman and J. M. Coxon-Blackie.
2. Modern Organic Reactions - H.O. House – Benjamin
3. Some Modern methods, of Organic Synthesis - W. Carruthers – Cambridge University Press.
4. Application of Organotransition Metals in Organic Synthesis - S.G. Davies.
5. Principles and Applications of Organotransition Metal Chemistry – J. P. Collman, L. S. Hegedus, J. R. Norton & R. C. Finke.
6. Organotransition Metal Chemistry – R. F. Heck.
7. Synthetic Coordination and Organometallic Chemistry- A. D. &Kharisov, B. I.
8. Palladium in Organic Synthesis – Tsuji, J. Palladium in Heterocyclic Chemistry: A Guide for the Synthetic Chemist- Li, J. J. & Gribble, G.W.
9. Heterocyclic Chemistry - J. A. Joule & K. Mills.
10. Heterocycles in Synthesis – A. I. Meyers.

Advance Organic Special-IV (45L) CHM21126

Unit-I: Advanced Heterocyclic Chemistry (20L)

Nomenclature of normal and fused heterocycles. Reactivity and synthesis of pyrimidine, pyridazines, pyrazines, purines, pteridines with and without oxygen and/or sulfur atoms, and their role in biological systems. Introduction to chemistry of azepins, oxepins, thiepins and their analogues; phosphorous and selenium containing heterocycles with the use of modern reagents. ANRORC and Vicarious nucleophilic substitutions in heterocycles.

Unit-II: Physical Organic Chemistry and Medicinal Chemistry II (25L)

Physical Organic Chemistry: MO treatment of acyclic and cyclic conjugated systems; Huckel's rule and concept of aromaticty, annulenes, heteroannulenes, fullerenes (C60), alternate and non-alternate hydrocarbons, antiaromaticity, pseudo-aromaticity, homo-aromaticity; graphical methods Frost diagram. Huckel treatment – applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene, Hammett equation and its modifications.

Medicinal Chemistry-II: Anti-bacterial drugs: Discovery of penicillin, Mechanism of action, Structure-activity relationship, Drug resistance, Role of clavulinic acid, New generation antibiotics. Anti-viral drugs: Discovery, Mechanism of action, Structure-activity relationship, Anti-cancer drugs: Introduction, examples and mechanism of action, PDT. Drugs working on cholinergic receptors: Introduction, examples and mechanism of action. Drugs working on adrenergic nervous system: Introduction, examples and mechanism of action. Opoid analegesics. Ant-ulcer drugs.

Reference Books:

1. Advanced Organic Chemistry - J. March. Physical Organic Chemistry – J. Hine.

2. Organic Chemistry - J. B. Hendrickson, D. J. Cram & J. H. Hammond; 3rd edition.
3. Organic Chemistry – J. Clayden; N. Greeves; S. Warren & P. Wothers.
4. Organic Reaction Mechanics- A. Gallego, M.Gomer& Sierra, M.A
5. Physical Organic Chemistry - N. S. Isaacs - Longman.
6. Hammett equation - C. P. Johnson
7. Organic Chemistry of Drug Design and Drug Action (3^{rd} Edition)- R. Silverman
8. Introduction to Medicinal Chemistry (6^{th} Edition)- G. L. Patrick

Advance Special Practical II **CHM22127**

Physical Chemistry

1. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions indifferent units (J molecule-1 kJ mol-1, cm-1, eV).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2- propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.
4. Determine the amount of iron present in a sample using 1, 10-phenathroline.
5. Kinetics of decomposition of benzene diazonium chloride.
6. Conductometric study of the kinetics of saponification of ethyl acetate.
7. Determination of transport numbers of Cu^{2+} and $SO4^{2-}$ by Hittorf's method.
8. Conductometric titration of triple mixture (HCl+NH4Cl+KCl) with (i) NaOH and (ii) $AgNO_3$.

Inorganic Chemistry Practical

1. Synthesis and structural characterization (IR, electronic spectra and magnetic susceptibility) of $[Ni(py)_4(NCS)_2]$. (b) Synthesis of a series of Ni(II) complexes (with ligands of varying ligand field strength), electronic spectral interpretation and calculation of various ligand-field parameters.
2. Synthesis and structural characterization (IR, Electronic spectra) of the cis- and trans isomers of $[Co(en)_2Cl_2]$
3. Synthesis and characterization (IR and PMR & CMR) of $[Al(acac)_3]$ 1. Synthesis, purification by sublimation and structural characterization (IR and electronic spectra) of ferrocene.
4. Acetylation of ferrocene and separation of the acetyl derivative by column chromatography.

Organic Chemistry Practical

1. Synthesis, separation and identification of organic mixtures containing up to three components.
2. Preparation of organic compounds involving several stages, characterization of intermediates and final products by IR and NMR spectroscopy.
3. Techniques of organic chemistry: Special practical's involving steam distillation, photo-isomerization and thin layer chromatography etc.

Reference Books:

1. Vogel's Text Book of Practical Organic Chemistry (5th Edition)
2. A Handbook of Organic Analysis: Qualitative and Quantitative (4th Edition) - Clarke

Project Work and Dissertation-II **CHM25128**

Course Content:

Chemistry is the science of matter, especially its properties, structure, composition, behavior, reactions, interactions and the changes it undergoes. Chemistry is sometimes called 'the central science' because it connects physics with other natural sciences such as astronomy, geology and biology. On completion of 5th Semester of B.Sc. Chemistry students will be acquainted with advance knowledge in Chemistry both theoretically and practically. Students are supposed to choose a research project allied to their expertise and chemical sciences. Students are expected to carry on the chosen research project and note down observations to reach out a possible scientific inference regarding the chosen project. On the completion of project work, students should submit their 'dissertation'.