# Curriculum Under

**National Education Policy**

COURSE STRUCTURE

**FOR**

# MASTER OF SCIENCE

# (CHEMISTRY)

**2026-27**

**Program Structure for 2-year Postgraduate Programs with Exit Option**

**Department of Chemistry**

**1st Year of PG curricular structure for 2-year PG Programmes (3+2)**

| 1st Year | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| SEMESTER I | | | | | | | | |
| **S.No** | **Type of Course** | **Code** | **Title of the Course** | **Contact Hours Per Week** | | | | **Total Credits** |
| | | | | **L** | **T** | **P** | **C** | |
| 1 | CC | CHM430 | Physical Chemistry I | 3 | 1 | 0 | 4 | |
| 2 | CC | CHM431 | Inorganic Chemistry I | 3 | 1 | 0 | 4 | |
| 3 | CC | CHM432 | Organic Chemistry I | 3 | 0 | 1 | 4 | |
| 4 | DSE/MDE | CHM433 / CHM434 | To be chosen from pool of discipline specific elective courses/ elective courses of other disciplines/ SAWYAM MOOC courses approved by the department<br><br>Mathematical and Computational Chemistry / Chemical Biology | 3 | 0 | 1 | 4 | |
| 5 | RM | CHM435 | Research methodologies in Chemistry | 2 | 1 | 1 | 4 | |
| 6 | SEC(Hands-On Training) | CHM436 | Advance Chemistry Lab I | 0 | 0 | 2 | 2 | |
| 7 | AEC | | Foreign Language-I | 2 | 0 | 0 | 2 | |
| 8 | SEC | | Career Development Course I (Soft Skill / Soft Skill and Aptitude Course) | 1 | 0 | 0 | 1 | |
| **Semester Credits** | | | | | | | **25** | |

| SEMESTER II | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 9 | CC | CHM501 | Physical Chemistry II | 3 | 1 | 0 | 4 | |
| 10 | CC | CHM502 | Inorganic Chemistry II | 3 | 1 | 0 | 4 | |
| 11 | CC | CHM503 | Organic Chemistry II | 3 | 1 | 0 | 4 | |
| 12 | DSE | CHM504/CHM505 | To be chosen from pool of discipline specific elective courses/ elective courses of other disciplines/ SAWYAM MOOC courses approved by the department/ Group theory and spectroscopy / Supramolecular Chemistry | 3 | 0 | 1 | 4 | |
| 13 | MDE | CHM506 | To be chosen from pool of discipline specific elective courses/ elective courses of other disciplines/ SAWYAM MOOC courses approved by the department/ Fundamental of Nano-science | 3 | 1 | 0 | 4 | |
| 14 | SEC(Hands-On Training) | CHM507 | Advance Chemistry Lab II | 0 | 0 | 2 | 2 | |
| 15 | AEC | | Foreign Language-II | 2 | 0 | 0 | 2 | |
| 16 | SEC | | Career Development Course I (Soft Skill / Soft Skill and Aptitude Course) | 1 | 0 | 0 | 1 | |
| **Semester Credits** | | | | | | | **25** | |
| **Exit option with Post-Graduate Diploma after the first year or two semesters with the completion of courses equivalent to 44 credits** | | | | | | | | |

## 2nd Year of PG curricular structure for 2-year PG Programmes

## One-year PG Programme after completion of Four-Year UG Programme (4+1)

### PG Curricular Structure with Coursework & Research

| 2nd Year | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **SEMESTER III** | | | | | | | | |
| **Sr. No** | **Type of Course** | **Code** | **Title of the Course** | **Contact Hours Per Week** | | | | **Remarks** |
| | | | | **L** | **T** | **P** | **C** | |
| 1 | CC | CHM510 | Modern methods of spectroscopy | 3 | 1 | 0 | 4 | |
| 2 | CC | CHM513/CHM514 / CHM515 | Principles of Catalysis and Catalytic Processes / Chemistry of Metal-Carbon complexes /Chemistry of drug design | 3 | 1 | 0 | 4 | |
| 3 | CC | CHM516 | **Spectroscopic methods of chemical analysis** | 2 | 1 | 0 | 2 | |
| 4 | DSE/MDE | CHM517/CHM518 | To be chosen from pool of discipline specific elective courses/ elective courses of other disciplines/ SAWYAM MOOC courses approved by the department/ Molecular crystal structure determination/ Inorganic Materials & Medicine | 3 | 1 | 0 | 4 | |
| 5 | Research | CHM520 | Dissertation -1 | 0 | 0 | 6 | 6 | |
| 6 | FP/ RP/ INT/ OJT | CHM521 | **Internship** | 0 | 0 | 2 | 2 | |
| | SEC | | Career Development Course I (Soft Skill / Soft Skill and Aptitude Course) | 1 | 0 | 0 | 1 | |
| | | | | | | | | |
| **Semester Credits** | | | | | | | **23** | |
| **SEMESTER IV** | | | | | | | | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1 | CC | CHM525/CHM526 | Quantum Chemistry and quantum dynamics / Synthetic strategies of smart materials | 3 | 1 | 0 | 4 | |
| | CC | CHM527 | **Advance Spectroscopy Lab.** | 0 | 0 | 2 | 2 | |
| 2 | DSE/MDE | CHM528/CHM529 | To be chosen from pool of discipline specific elective courses/ elective courses of other disciplines/ SAWYAM MOOC courses approved by the department/<br><br>Nano-biotechnology and nano-medicine/ Simulation techniques in chemistry | 3 | 1 | 0 | 4 | |
| 3 | ED | CHM530 | Entrepreneurship | | | | 2 | |
| 4 | Research | CHM531 | Dissertation-II | | | 12 | 12 | |
| | | | | | | | | |
| | | | | | | | | |
| **Semester Credits** | | | | | | | **22** | |

Total credit for 2-year M.Sc. (Chemistry) = **95**

# Curriculum Under National Education Policy

**Syllabus**

**FOR**

## MASTER OF SCIENCE

## (CHEMISTRY)

**Department of Chemistry**

**Adamas University**

**2026**

# Semester-I

**CC- CHM430** **L-T-P-C: 3-1-0-4**

**Physical Chemistry I**

**Unit 1: Classical Thermodynamics (10L)**

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 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 (13L)**

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.

**Unit-5: Analytical tools for Characterization of Complexes (10 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

**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.


| | | | | | |
|---|---|---|---|---|---|
| CHM436 | Advance Chemistry Lab I | 0 | 0 | 2 | 2 |

**A. Spectrophotometric study:**

1. To test the validity of Beer-Lambert's law and hence determination of unknown concentration in a solution
2. Study the effect of ionic strength on the reaction: $K_2S_2O_8 + KI \rightarrow 2K_2SO_4 + I_2$; spectrophotometrically.
3. Autocatalytic reaction: reaction of $KMnO_4$ with oxalic acid
4. Spectrophotometric determination of Iron in different mixtures.
5. Determination of coordination number of metal ions in a metal complex by Job's continuous method.

**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. Complexometric and iodometric study**

1. Determination of amount of $Ca^{2+}$ in commercial milk powder by complexometric method.
2. Determination of iodine content in commercial salt by iodometric method.
3. Estimation of Cu(II) and Zn(II) present in a mixture by iodometric titration.

**Reference Books**

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

## CC CHM431

## Inorganic Chemistry I (45L) L-T-P: 3-1-0

**Unit-1: Bonding in Transition Metal Complexes (20 L)**

Crystal field theory, Splitting of d orbitals in different crystal fields. Octahedral site preference energy, tetragonal distortion and Jahn Teller effect. Preference of Geometry of Metal Complexes with different ligand. 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.

**Unit-3: Magnetic property of coordination complexes (10L)**

Magnetism and magnetic moments, Spin only magnetic moments and their correlation with effective magnetic moments, Orbital contribution towards magnetic moment and its quenching in crystal field, Exchange interaction in metal complexes, Introduction to magnetic properties to Lanthanides, Magnetic exchange coupling, Spin-cross over phenomena, Photomagnetism.

**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*

## CC-CHM432

## Organic Chemistry I (45L) L-T-P: 3-0-1

**Unit-I: Physical Organic Chemistry (10L)**

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.

**Unit-II: Photochemical reaction (10L)**

Photolysis of carbonyl compounds and nitrites: Norrish Type I, Norrish Type II, α-cleavage, Barton reaction, photoreduction, photoexcitation, photorearrangement reactions (Photorearrangemnt reaction of cyclohexanones, cyclohexadienone and α-tropolone methyl, Di-π-methane, photoisomerisation and photodimerisation), cycloadditions of benzene and its derivatives.

**Unit-III: 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. Application of Diels-Alder reaction in natural product synthesis; synthesis of strychnine, cortisone, cholesterol, and indomethacin, 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. Organic Photochemistry - J. W. Coxon& B. Halton,
2. Elements of Organic Photochemistry - D. O. Cowan & K. L. Drisco,
3. Pericyclic Chemistry – S. M. Mukherjee.
4. Frontier Orbitals and Organic Chemical Reactions – I. Fleming
5. Physical Organic Chemistry - N. S. Isaacs - Longman.


**Unit-IV: Lab- Extraction, small heterocycle Synthesis:**

1. Natural product extraction (caffeine, nicotine, casein etc.) etc.
2. Heterocycle Synthesis:
    a) Synthesis of benz-oxazole from o-amino phenol derivatives,

b) Synthesis of phthalazine derivative from phthalic anhydride,
c) Synthesis of pyrazolone derivative from phenyl hydrazine,
d) Synthesis of coumarin derivative from resorcinol,
e) Synthesis of indole and carbazole derivative from phenyl hydrazine,
f) Synthesis of barbituric acid etc.

**Reference Books:**


1. Das, S.C. Advanced Practical Chemistry, Sixth edition,
2. Mukherjee, G.N. University handbook of undergraduate chemistry experiments.


**DSE- CHM433** **L-T-P-C:2-0-2-4**

**Mathematical and Computational Chemistry** **CHM23129**

**Unit-I: Mathematics-Review** **(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: Programming** **(10)**

Computer programming in FORTRAN/Python/C++. 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.


## DSE-CHM434

## Chemical Biology L-T-P: 3-1-0

### Unit I: Introduction (15L)

Background and definition of chemical biology, overview of chemical biology and its' importance, allied fields and their link with chemical biology, Proteins and Amino Acids: alpha-Amino Acids, other amino acids and their importance, isoelectric point, preparation of amino acids, reactions of AA, peptide bond formation, reagents-reactions, solid phase peptide synthesis, peptides and proteins, overview of protein structure, protein-protein interactions, its's application in biology.

### Unit II: Biomolecular-drug interaction (15L)

Key discoveries in the field of chemical biology, few examples and journey through those discoveries, the use of unusual amino acids to probe biomolecular conformation, the use of novel fluorescence probe and applications, small molecule kinase inhibitors, GTP analogues as potential regulators for microtubule dynamics.

### Unit III: Bioorthogonal reaction and its' application in Chemical Biology (15L)

Foundational Concepts of Bioorthogonal reaction; Click Chemistry Principles Reaction Mechanism, Reaction Conditions; Bioorthogonal Reaction Types, Applications of Bioorthogonal Reactions; Biomolecule Labeling, Protein Modification, Cell Imaging, Techniques for Application in Live Cells and In Vitro; In Vitro Labeling, In Vivo Labeling, Cell-Based Assays.

**Textbook:**

1. Chemical Biology: From Small Molecules to Systems Biology and Drug Design (Willey), Editor(s): Profs. Stuart L. Schreiber, Tarun M. Kapoor and Günther Wess, Nature Chemical Biology, 2010, 6, 847-853.

## CHM435: Research methodologies in Chemistry L-T-P: 2-1-1

**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.

# Semester-II

**CC- CHM501** **L-T-P-C: 3-1-0-4**

**Physical Chemistry II**

**Unit-1: Quantum Mechanics-I (12L)**

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. Helmann-Feynmann Theorem.

**Unit-II: Quantum Mechanics -II (18L)**

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.

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

**Unit-III: Statistical Thermodynamics (15L)**

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 (15L)**

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.

## Inorganic Chemistry II (45L) CHM502 L-T-P: 3-1-0

**Unit-I: Kinetics and Mechanism of Substitution Reactions (15 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 (15 L)**

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-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 (15 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.

**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*

| | | | | | |
|---|---|---|---|---|---|
| CHM507 | Advance Chemistry Lab II | 0 | 0 | 2 | 2 |

**Lab Course Content:**

1. Optimization of GC Analysis: the van Deemter Plot
2. Analysis of the Components in an Over-the-Counter Analgesic Drug using Ultraviolet Spectroscopy.
3. Determination of Iron in a Vitamin Tablet by Ultraviolet-Visible Spectroscopy
4. Determination of iron content in various soils.
5. Estimation of $Fe^{3+}$ and $Cr^{3+}$ in a mixture by dichromatometric method.
6. Determination of $Mg^{2+}$ and $Fe^{3+}$ in blood samples by spectrophotometric and complexometric method.

**Reference Books:**


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


## CC-CHM503

## Organic Chemistry II L-T-P: 3-1-0

**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.

**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 – R.O.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.


**DSE- CHM504 L-T-P-C:3-0-1-4**

## Group Theory and Spectroscopy

**Unit 1: Group Theory (15 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 (10 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. FT IR – principles and instrumentation, Fourier transformation and instrumentation.

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.

**Unit 4: Resonance Spectroscopy (NMR & ESR) (10 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. Principles of FT NMR and 2D-NMR.

**Lab:**

1. Estimation of Quinine sulphate by Fluorimetry
2. Determination of the Relative Quantum Yield of Rhodamine B
3. Measure the absorption and emission spectra of anthracene and verify the mirror image rule.
4. Study of quenching of fluorescence
5. Analysis of NMR spectra to predict the structures of organic molecules.

**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;


**DSE-CHM505**

**Supramolecular Chemistry L-T-P: 3-1-0**

**Unit-I**: 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,

**Unit II**: Liquid crystals and supramolecuar polymers, polymer-surfactant interaction. New molecular receptors: crown ethers, siderophores, cyclophanes, cyclodextrin and their application in specific recognition processes.

**Unit III:** Supramolecular reactivity and catalysis, switching devices, self-assembly of supramolecular aggregates, crystal engineering and drug delivery.

**Reference Books:**


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


## Fundamental of Nano-science CHM506 L-T-P=3-1-0

**Unit-I: Nanomaterials: Inorganic and Biomaterials**

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 behaviour changes, Surface Plasmon Resonance (SPR), Direct and Indirect Transitions: Discussions on Nanoclusters and Nanowires; Metal, Metal Oxide, semiconductor nanoparticles, Carbon Nanotubes, Carbon nanodots, 2-D Nanopatterns and Self-assembled Monolayers on Inorganic Substrates; Mesostructured and Mesoporous Materials; Inorganic-Organic and Inorganic-Polymer Nanocomposite Materials; Polymeric nanoparticles, 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 and Catalysis Fields**

Advantages of nano electrical and electronic devices, Lighting and Displays, Light Emitting Diodes, Solar cells and Solar Panels, 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, 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).


# SEM-III

## Coursework with research

**Modern methods of spectroscopy (60L) CHM510** **L-T-P: 3-1-0**

**Unit 1: Fundamentals of spectroscopy:**
**(12L)**

Electromagnetic radiation and its interactions with matter; Atomic and Molecular energy levels and their symmetry; Applications of group theory for interpreting spectroscopic results: symmetry, direct product, integrals and selection rules; Angular momentum: spin-orbit coupling; Transition moment

integral; Spectroscopic line broadening and lamb-dip spectroscopy; Difference between condensed phase and gas phase study; Effect of hydrogen bonding; Single and double slit experiment; Michelson's Interferometry; The Stern-Gerlach experiment and spin quantum number

**Unit 2: Instrumentations and coupled techniques: (10L)**

Fourier transformation and its instrumentations; Effusive beam and molecular beam techniques: Isolated molecules and molecular clusters; Liquid jet techniques; Photon and ion detector; Position sensitive (2-Dimension) detector; Basic data analysis procedure; Measurement techniques in atmospheric chemistry, Time of flight (TOF) mass spectrometry, Time-resolved techniques

**Unit 3: Laser Spectroscopy: Principles and Applications: (10L)**

Types of light-source; Basic concepts of Lasers: types, principle of operations and applications; Synchrotron radiation and free electron lasers; Resonance Enhanced Multiphoton ionization (REMPI); Laser induced fluorescence spectroscopy (LIF); Cavity Ring Down spectroscopy (CRD); Photoelectron-Photoion Coincidence Spectroscopy (PEPICO); Double resonance Pump-Probe spectroscopy; Velocity map imaging (VMI); Collision-induced-dissociation (CID) techniques

**Unit 3: Electronic spectroscopy of isolated polyatomic molecules: (8L)**

Orbital and states; Potential energy surfaces; Radiative and non-radiative processes of isolated molecules and clusters; Molecular interpretation of non-radiative transitions: Internal conversion and Intramolecular vibrational redistribution (IVR); Vibrational structures in electronic transitions: Normal modes and their symmetry; Laser-Induced-Fluorescence spectroscopy: Single vibronic level fluorescence; Franck-Condon factor; Experimental spectral analysis with the help of quantum chemical calculations and group theory, test case: Vibronic spectra of Benzene, The Herzberg–Teller and Dushinsky effect

**Unit 4 : Fluorescence spectroscopy: Probing the Molecular World (10L)**

Types of electronic transitions in polyatomic molecules; Probability of transitions; Oscillator strength; Selection rules; Franck–Condon principle; Jablonsky diagram; Lifetimes and quantum yields; Fluorescence and other de-excitation processes of excited molecules; Fluorescent probes; Molecular fluorescence as an analytical tool; Ultimate spatial and temporal resolution: femtoseconds, femtoliters, femtomoles and single-molecule detection, Steady-state fluorescence intensity, Emission spectra, Excitation spectra, Stokes shift, Effects of molecular structure and functional group (-OH, -OR, -NHR, $-NH_2$, >C=O, $-NO_2$) on fluorescence; Internal heavy atom effect; Compounds undergoing photoinduced intramolecular charge transfer (ICT) and internal rotation; Environmental factors affecting fluorescence; Fluorescence quenching: Static and dynamic, Photoinduced electron transfer; Formation of excimers and exciplexes; Photoinduced proton transfer; Determination of the excited-state

pK*; Time-resolved methods; pH dependence of absorption and emission spectra; Excited state energy transfer; Steady-state and time-resolved fluorometric techniques; Resonance energy transfer and its applications; Effect of polarity on fluorescence emission

**Unit 6: Photoelectron Spectroscopy:** **(10L)**

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. Banwell, C. N. (1983). *Fundamentals of molecular spectroscopy* (3rd ed). McGraw-Hill.
2. Bernath, P. F. (2016). *Spectra of atoms and molecules* (Third edition). Oxford University Press.
3. Hollas, J. M. (2004). *Modern spectroscopy* (4th ed). J. Wiley.
4. Ellis, A. M., Fehér, M., & Wright, T. G. (2005). Electronic and photoelectron spectroscopy: Fundamentals and case studies. Cambridge University Press.
5. Valeur, B. (2001). Molecular Fluorescence Principles and Applications.


## Principles of Catalysis and Catalytic Processes CHM513 L-T-P: 3-1-0

**Unit-1:** **(8L)**

**Introduction to Catalysis:** Definition, Types, Surface and adsorption, Process of adsorption, Physisorption, Chemisorption, Adsorption isotherms, Kinetics and mechanisms of catalytic reactions: Langmuir-Hinshelwood Kinetics, Eley-Rideal Kinetics, Mars-Van Krevelen Mechanism

**Unit-2:** **(12L)**

**Heterogeneous Catalysis:** Chemistry of heterogeneous catalysis: Surface bonds, Catalyst geometries, Active sites, Activation energy, Catalytic activity, Promoters, Stabilizers, Catalyst deactivation, Chemisorption on metals, metal oxides and semiconductors; Catalyst supports, Solid acids and bases as catalysts, Nanoporous materials.

**Unit-3:** **(10L)**

**Preparation and Characterization of Catalysts:** Selection, design and preparation of catalysts: Catalyst formulations and preparation, Catalyst supports, Supported catalysts by impregnation, Co-precipitation; Catalyst characterization: Chemical composition, Phase structure, Physical texture,

Surface area and pore volume distribution; Catalytic activity, selectivity and stability under operating conditions.

**Unit-4: Homogeneous Catalysis and Biocatalysis:** Catalysis by acids, Homogeneous Catalysis by organometallic compounds, Ziegler-Natta catalyst, Wilkinson catalyst; Enzyme catalysis: : Hallmarks of an enzyme catalyst: catalysis, specificity, regulation – Origins of enzyme catalytic power: proximity and orientation effects, contribution by electrostatics, metal ions in catalysis, acid-base catalysis Michaelis–Menten mechanism, Lineweaver–Burk equation, Enzyme activity, Performance criteria for process schemes. Catalytic mechanisms: Acid-base catalysis, electrostatic catalysis, metal-ion catalysis, covalent catalysis – Mechanism of action of enzymes: The Fisher template model (lock and key model), Induced fit model, Covalent catalysis – Factors affecting enzyme activity

**Unit-5: Catalytic processes:** Environmental protection, Energy processing, Energy conversion and storage, Biomass conversion, Biodiesel, Fine chemical synthesis, Synthetic fuels, pharmaceutical applications of biocatalysts, Future directions. Applications: Expert lectures, online seminars – webinars.

**References:**


1. Julian R.H. Ross, Heterogeneous Catalysis: Fundamentals and Applications (I Edition) (2011), Elsevier

2. Andreas S. Bommarius, Bettina R. Riebel, Biocatalysis (2004), WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

3. Piet W.N.M. van Leeuwen, Homogeneous Catalysis: Understanding the Art (2004), Kluwer Academic Publishers

4 B. Viswanathan, S. Sivasanker, A.V. Ramaswamy, Catalysis: Principles and Applications (2002), CRC Press, Taylor and Francis Group.

5 I. Chorkendorff, J.W. Niemantsverdriet, Concepts of Modern Catalysis and Kinetics (2003), WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

6. Roger Arthur Sheldon, Isabel Arends, Ulf Hanefeld, Green Chemistry and Catalysis (2007), WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

7. Jens Hagen, Industrial Catalysis: A practical approach (2015), WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

8. D. K. Chakrabarty, B. Viswanathan, Heterogeneous Catalysis (2008), New Age Science Ltd.

9. Jens K. Norskov, Felix Studt, Frank Abild-Pedersen, Thomas Bligaard, Fundamental Concepts in Heterogeneous Catalysis (2014), John Wiley& Sons, Inc.

10. Sumit Bhaduri, Doble Mukesh, Homogeneous Catalysis: Mechanisms and Industrial Applications (2000), John Wiley & Sons, Inc.


## Chemistry of Metal Carbon Complexes CHM 514 L-T-P: 3-1-0

**Unit I:** 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. Dioxygen and dinitrogen, nitrosyl, tertiary phosphines and arsines as ligands. Complexes of π-donor ligands: Transition metal alkenyls, alkynyls, carbenes, Fischer carbenes, Schrock, carbenes, complexes with N-heterocyclic carbenes (NHCs), 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.

**Unit II:** Transition metal Compounds with M-H bonds: Metal hydrides (classical and nonclassical). Agostic interaction. Application of NMR in studying hydrido complexes.

**Reaction of organometallic complexes:** Small molecules activation. Organometallics in organic synthesis C-C bond coupling reactions (Heck, Sonogashira, Suzuki-Miyaura, Stille etc) Reduction using transition metal hydrides, asymmetric hydrogenation.

**Unit III:** Catalysis by organometallic compounds

Hydroboration, Alkene metathesis**,** Zeigler-Natta polymerization reaction and their applications in various industrial processes (e.g., petrochemical industry, pharmaceuticals)

## Chemistry of drug design CHM515 L-T-P: 3-1-0

**Unit I: Drug design principle (15L)**

Introduction to Drug Discovery and Development, Physicochemical principles of drug action; Partition coefficients; Receptor-Effector theories; Role of second messengers in drug action; Methods of receptor isolation, Characterization and modeling; Principles of drug design: Random screening, Analogue synthesis, Rational design, Combinatorial libraries; Enantiopure drugs and regulatory implications; Theoretical approaches: QSAR, Topliss Tree, MSA, CoMFA.

**Unit II: Drug metabolism (15L)**

Target Identification: Understanding the biological targets (e.g., enzymes, receptors, DNA) and their role in disease, Lead Discovery and Optimization: Finding and refining molecules with desired activity. Stereochemistry and Pharmacophore Mapping: Understanding the importance of molecule shape and spatial arrangement in drug-target interactions. ADME and Pharmacokinetics/Pharmacodynamics (PK/PD): Studying how drugs are absorbed, distributed, metabolized, and excreted, and their effect on the body. Drug likeness and Lipinski's Rule of 5: Predicting the drug-likeness of new compounds based on their physicochemical properties. Detoxification of diverse drug classes; dose formulation

**Unit III: Synthesis and mechanism of action of various drugs (15L)**

Anti-bacterial drugs: Discovery of penicillin, Synthesis and mechanism of action, Structure-activity relationship, Drug resistance, Role of clavulinic acid, New generation antibiotics. Anti-viral drugs: Discovery, Synthesis and mechanism of action, Structure-activity relationship, Anti-cancer drugs: Introduction, examples, synthesis and mechanism of action, PDT. Neuroactive Drugs: Neurons and neurotransmitters; Brain-related disorders and chemotherapy; drugs interacting with cholinergic, adrenergic, dopaminergic and histaminic receptors and receptor-subtypes; Opoid analegesics; Ant-ulcer drugs; Drug delivery: Passive, assisted and vector-based delivery of conventional and genetic drugs; Tissue-specific delivery of antitumor agents.

**Reference Books:**

1. Medicinal Chemistry: A Biochemical Approach, Thomas Nogrady
2. Principles of Medicinal Chemistry, William O. Foye
3. The Pharmacological Basis of Therapeutics: Goodman and Gilman
4. Introduction to Drug Metabolism, G. Gordon Gibson and Paul Skett

## Molecular crystal structure determination CHM517 L-T-P: 2-0-2

**Unit I:** Crystal and lattice, 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,

**Unit II:** Process of crystallizations, crystal form, habit, defect, different methods for the growth of single crystal. Crystal protection from environment. Hydrothermal, solvothermal, diffusion, layered crystallization methods.

**Unit III:** 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.

### Molecular crystal structure determination: Lab.

1. Crystal formation from different methods
2. X-ray data collection and analysis
3. X-ray Structure solution using Wingx, SHELX, and Apex
4. Structure elucidation and analysis in graphical tools (Mercury, Diamond, ORTEP etc)

## Inorganic Materials and Medicine CHM518 L-T-P: 3-1-0

**Unit I: Life with Oxygen**

Dependence of life on oxygen. Fundamentals related to dioxygen and need for its activation. Various biological activities and applications.

**Unit II: Metals and Medicine**. History of metals in medicines. Overview of metals used in the ancient times and today as therapeutic and diagnostic agents. Rosenberg's accidental landmark discovery of cisplatin as blockbuster anticancer drug. Mechanistic action of the drug and the current status.

**Unit III: Electron Transfer Process**

Contribution of Prof. Henry Taube for his outstanding work on the mechanisms of electron transfer reactions, especially in metal complexes. Various electron transfer processes and their application in different life processes.

**Unit IV: Catalysis and Sustainability**

Fundamental role of catalyst and its design towards critical role. Catalytic activities of few selected and important catalysts and their industrial applications. Recent development on Green Chemistry for chemical synthesis and sustainable chemical processes

**Unit V: Inorganic Materials**

Introduction of new generation materials, such as network structures, molecular (nano)machines and molecular (nano) devices based on supramolecular chemistry and molecular self-assembly. Functional exploration of materials used for Magnetic, Optical, Conducting and Storage materials.

**Reference books:**


Concepts and Models of Inorganic Chemsitry, 3rdEdn., B. Douglas, D. McDaniel and J. Alexander, John Wiley, New York. 1993

Concepts and Models of Inorganic Chemsitry, 3rdEdn., B. Douglas, D. McDaniel and J. Alexander, John Wiley, New York. 1993

Supramolecular Chemistry, J-M. Lehn, VCH, Weinheim, 1995

Supramolecular Chemistry, J. W. Steed and J. L. Atwood, John-Wiley and Sons, Ltd., 2000

Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard & J. S. Valentine, Viva Books Pvt. Ltd., 2004.

Shriver and Atkins Inorganic Chemistry, 5thEdn., Oxford University Press, 2009.

Organotransition Metal Chemistry: From Bonding to Catalysis, 1stEdn., J. Hartwig, 2010

Molecular Magnetic Materials: Concepts and Applications, Editors(s): B. Sieklucka and D. Pinkowicz, Wiley-VCH, 2016

Molecular Magnetic Materials: Concepts and Applications, Editors(s): B. Sieklucka and D. Pinkowicz, Wiley-VCH, 2016


## Inorganic materials of Industrial Importance, CHM532 L-T-P: 3-0-1

**Unit I: Silicate Industries**

**Glass:** Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types

ofglasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass,fluorosilicate, coloured glass, photosensitive glass.

*Ceramics*: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

*Cements:* Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

**Unit II: Fertilizers:**

Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

**Unit III: Surface Coatings:**

Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plasticpaint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolyticandelectroless), metal spraying and anodizing.

**Unit IV: Batteries:**

Primary and secondary batteries, battery components and their role, Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery & Fuel cells, Solar cell and polymer cell.

**Unit V: Alloys:**

Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

**References Books:**


- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.

• R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.

• W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.

• J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.


**Course: Inorganic materials of Industrial Importance Lab**

**Course Content**

1. Determination of free acidity in ammonium sulphate fertilizer.
2. Estimation of Calcium in Calcium ammonium nitrate fertilizer.
3. Estimation of phosphoric acid in superphosphate fertilizer.
4. Determination of composition of dolomite (by complexometric titration).
5. Analysis of (Cu, Ni); (Cu, Zn) in alloy or synthetic samples.
6. Analysis of Cement.
7. Preparation of pigment (zinc oxide).

# Semester -IV

**Quantum Chemistry and Quantum Dynamics, CHM525** **L-T-P: 3-1-0**

**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** **(7)**

Rayleigh-Schrodinger perturbation theory for non-degenerate states (review). Degenerate perturbation theory-Stark effect. First and second order lifting of degeneracy. Variation method: Basis and applicability (review). Linear variation method- secular determinant.

**Unit-III: Theoretical aspects of spectroscopy- Quantum dynamics (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-I: Multi-electron system (15)**

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. Electron correlation. Multideterminantal wave function and CI. Brillouin's theorem. Rudiments of Density Functional Theory: Expectation Value calculation using density: Kohn-Hohnenberg Theorems; Kohn-Sham equation for the ground state of many body systems.

Lab:

Quantum Chemical calculation by using Gaussian16 software.

- Energy calculation
- Structure optimization
- IR spectrum
- Reaction path

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. Introduction to Quantum Mechanics: David J. Griffith,


**Synthetic Strategy of Smart Materials CHM526, L-T-P: 3-1-0**

**Unit I: Conventional methods**

Variety of inorganic (traditional to advanced) materials, Importance of Structural/refractory, Electronic and Bio-materials, Oxide superconductors and novel materials. Description of crystals, Bonding, Inorganuc structures, Silicates and Alluminosilicates, Polytypism, Nanocrystalline/amorphous solids.

**Unit II: Characterization techniques**
X-ray diffraction, Electron and Neutron Diffraction, AFM / SEM / TEM, Thermal(TG / DTG / DTA / DSC) and BET technique, XAS, EPR, IR, UV- Visible.

**Unit III: Conventional techniques**
Powder mixing, Fusion, Precipitation from solution, modern need for improved synthetic routes, Crystal growth and thin film techniques.

Sol-gel synthesis:
Colloids, Cation hydrolysis and sol formation, Gel precipitation, Sol-Gel process for colloids, synthesis and Physical properties of Metal alkoxides, Development of Sol-Gel process from alkoxides, derived coatings, fibers and monodispersed submicron / nanostructured oxide powders, Ormosils, Sialons.

Hydrothermal synthesis:
Forced hydrolysis at elevated temperatures and pressures, Hydrothermal reactions using salt solutions, Metal reactants and reactions involving phase transformation.

Special reactions:
Topochemical reactions, Intercalation reactions, Ion-exchange method, Molten Salt method, Electrochemical methods, Chemical vapour deposition, Reactions at high pressures, Intergrown structures and microwave digestion reactions.

**Unit-IV: Non-aqueous liquid phase reactions**
Reactions of chlorosilanes with ammonia, amines in liquid phase, Synthesis of non-oxide materials: Silicon Nitride, Metal-Borides, Carbides, Nitrides, Fluorides: Metal-Silicides, Phosphides, Sulfides and related materials.

## Nano-biotechnology and nano-medicine CHM528, L-T-P: 3-1-0

**Unit I: Introduction to various biomaterials and their properties (15L)**

Definition of nanomaterials and types of nanomaterials used for the biomedical applications: inorganic nanomaterials (gold, silica, silver, graphene oxide, carbon nanotubes, quantum dot, up-conversion nanoparticles, iron oxide nanoparticles), organic nanomaterials (peptide, polymers, hydrogel, dendrimer), detailed surface properties analysis of the biomaterials and their interaction study towards the cell and their in vitro cell and in vivo toxicity assessment, limitation of the current chemotherapeutics.

**Unit II: Characterization techniques of various nanomaterials and their surface engineering (15L)**

Various characterization techniques for biomaterials: UV-Vis spectroscopy, FT-IR spectroscopy, NMR spectroscopy, dynamic light scattering, photoluminescence spectroscopy, transmission electron microscopy (TEM), high performance liquid chromatography, fluorescence and confocal microscopy; surface modification of the nanomaterials: covalent vs noncovalent modification, chemical modification, noncovalent coating with polymer, protein, biomolecules; biocompatibility test.

**Unit III: Nanomaterials for various biomedical application and associated biochemical assay (15L)**

Various biomedical application of the nanomaterials: drug delivery, gene and siRNA delivery, photodynamic and photo thermal therapy, in-vitro cell and in-vivo imaging, anticancer, antibacterial and antifungal activity, self-therapeutics nanomaterials towards development of nanomedicine, mechanistic insight of the drug delivery systems, various cell based biochemical assays, tumor model for studying the in vivo application.

**Text Books:**

1. Basu Bikramjit, Biomaterials Science and Tissue Engineering, Cambridge University Press; First edition (2017), ISBN-10: 1108415156.

**Reference Books:**

1. William R Wagner, Shelly E. Sakiyama-Elbert, Guigen Zhang, Michael J. Yaszemski, Biomaterials Science: An Introduction to Materials in Medicine, Academic Press Inc; 4th edition (2020), ISBN-10: 012816137X.

**Self-Learning Material:**

1. Prof. Bikramjit Basu, IIT Kanpur, https://nptel.ac.in/courses/113/104/113104009/ .

**DSE: Simulation in Chemical System, CHM529, L-T-P: 3-1-0**

**Unit 1: Chemical Kinetics:**

Simulation of simultaneous differential equations. Euler and Runge Kutta method.

**Unit 2: Molecular Dynamics:**

Potential energy surfaces and intermolecular interactions; Bonded and non-bonded interactions Classical and polarizable force fields, Energy calculations using molecular mechanics. Simple applications of molecular modelling: Study of an assembly of atoms or molecules (clusters and/or bulk phases). Approximation of the total potential energy as the sum of pair potentials. Concept of large number of microstates, averages and basic principles of simulations. Study of cluster and bulk properties through simulations. Continuum models versus molecular models. Modelling of macromolecules: Study of self-organized assemblies, biomolecules like peptides, proteins, membranes and ion channels. Concept of hydrophobic and hydrophilic interactions.

**Unit 3: Monte Carlo Simulation:**

Introduction to Monte Carlo methods, Statistical mechanics applications, random number generation, algorithms to integrate equations of motion.

Brownian particle, Langevin model Equation of motion including thermal noise Conditional and thermal averages.

**Unit 4: Gillespie Algorithm**:

Monte Carlo simulation of chemical and biological reacting systems.

Optimization Algorithms:

Deterministic and stochastic optimization algorithms. Application in structure determination in static force field.

Lab:

1. Molecular Dynamics simulation.
2. Time series for reacting system: deterministic and stochastic simulations.
3. Noise calculation.
4. Optimization of simple atomic cluster system.

Reference:


1. D. Frenkel and B. Smit, *Understanding Molecular Simulation: From Algorithms to Applications*, 2nd edition, Academic Press
2. M.P. Allen and D.J. Tildesley, *Computer Simulations of Liquids*, Oxford Clarendon Press.
3. Gillespie D T 1976 *J. Comp. Phys.* **22** 403
4. Gillespie D T 1977 *J. Phys. Chem.* **81** 2340
5. Kirkpatrick K S, Gelatt C D and Vecchi M P 1983 *Science* **220** 671
6. Goldberg D E 1989 *Genetic algorithm in search, optimization and machine learning* (Reading, MA: Addison Wesley)


## Spectroscopic Techniques for chemical analysis (60L) L-T-P-C: 3-1-0-4 CHM535

**Unit 1: Analytical approach: (10L)**

Analytical Figures of Merit: Sensitivity, selectivity, resolution, Detection limit, quantification limit, Calibration curves and linearity, Signal-to-noise ratio (SNR)

Sampling and Sample Preparation: Gaseous, liquid, and solid samples, Matrix effects and sample compatibility, Dilution, digestion, extraction, and enrichment

Qualitative and Quantitative Analysis: Identification of unknowns via spectra, Calibration strategies (external, internal standard, standard addition), Multivariate data analysis

Error and Uncertainty in Spectroscopy: Sources of error (instrumental, operational, environmental), Propagation of uncertainty, Method validation: precision, accuracy, robustness

**Unit 2: Spectrophotometric Methods for characterization: (12L)**

Beer–Lambert Law and its limitations, Selection rules, Absorbance, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transitions, Quantitative analysis (Beer's law, calibration curves) Kinetics studies, drug assays, food additives Spectral Interpretation: $\lambda\_max$, molar absorptivity, bathochromic/hypsochromic shifts, Chromophores and auxochromes, The Nature of Electronic Excitations, The Origin of UV Band Structure, Principles of Absorption Spectroscopy, Instrumentation, Presentation of Spectra, Solvents, What is a Chromophore, The Effect of Conjugation, Effect of Conjugation on Alkenes, Woodward-Fieser Rules for Dienes, Carbonyl Compounds: Enones, Woodward's Rules for Enones, α, β-Unsaturated Aldehydes, Acids, and Esters, Aromatic Compounds, Effect of electron-releasing and electron-withdrawing Effects, Disubstituted Benzene Derivatives, Polynuclear Aromatic Hydrocarbons and Heterocyclic Compounds, Model Compound Studies, Visible Spectra: Color in Compounds, What To Look for in an Ultraviolet Spectrum: A Practical Guide

**Unit-3: Mass spectrometric analysis: (12L)**

Principles, instrumentation and applications of mass spectrometry; Methods of generation of ions in EI, PI, CI, FD and FAB and other techniques; Detection of ions, ion analysis, ion abundance, molecular ion peak, metastable peak, isotopes, Quasi-Equilibrium Theory; Fragmentation patterns of ions; Ionization Efficiency and Ionization Cross Section; Appearance energy, Bond dissociation energies and heats of formation; Tandem mass spectrometry; Applications of mass spectrometry to simple structural and mechanistic problems.

**Unit 4: IR Spectroscopy for Structural and Functional Group Analysis: (14L)**

The Infrared Absorption Process, Uses of the Infrared Spectrum, The Modes of Stretching and Bending, Bond properties and Absorption trends, Preparation of samples for infrared spectroscopy, What to look for when examining infrared spectra, Correlation Charts and Tables, Analysis of a spectrum for structural information: Hydrocarbon, Aromatic rings, Alcohols and phenols, Carbonyl compounds and carboxylic acid derivatives, Factors that Influence the C=O Stretching Vibration, Ethers, Sulphur and phosphorus containing compounds, Alkyl and Aryl Halides, Structure determination.

**Unit 5: Case Studies and Emerging Trends: (12L)**

Forensic applications, Quality control in pharmaceuticals, Environmental pollutant monitoring, Biospectroscopy and point-of-care diagnostics, Atmospheric measurement, Spectral database, Astrochemical measurement, and spectroscopy in space

**Reference books:**


1. Pavia, D. L., Lampman, G. M., Kriz, G. S., & Vyvyan, J. R. (2009). *Introduction to spectroscopy* (4th ed). Brooks/Cole, Cengage Learning.
2. Ellis, A. M., Fehér, M., & Wright, T. G. (2005). Electronic and photoelectron spectroscopy: Fundamentals and case studies. Cambridge University Press.
3. Kemp, W. (1991). Organic Spectroscopy. Macmillan Education UK
4. Gross, J. H. (2004). *Mass spectrometry: A textbook*. Springer.


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**Spectroscopic methods of chemical analysis (60L) L-T-P-C: 2-0-0-2**

**Unit 1: Analytical approach: (5L)**

Analytical Figures of Merit: Sensitivity, selectivity, resolution, Detection limit, quantification limit, Calibration curves and linearity, Signal-to-noise ratio (SNR)

Sampling and Sample Preparation: Gaseous, liquid, and solid samples, Matrix effects and sample compatibility, Dilution, digestion, extraction, and enrichment

Qualitative and Quantitative Analysis: Identification of unknowns via spectra, Calibration strategies (external, internal standard, standard addition), Multivariate data analysis

Error and Uncertainty in Spectroscopy: Sources of error (instrumental, operational, environmental), Propagation of uncertainty, Method validation: precision, accuracy, robustness

**Unit 2: Spectrophotometric Methods for characterization: (8L)**

Beer–Lambert Law and its limitations, Selection rules, Absorbance, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transitions, Quantitative analysis (Beer's law, calibration curves) Kinetics studies, drug assays, food additives Spectral Interpretation: $\lambda$_max, molar absorptivity, bathochromic/hypsochromic shifts, Chromophores and auxochromes, The Nature of Electronic Excitations, The Origin of

UV Band Structure, Principles of Absorption Spectroscopy, Instrumentation, Presentation of Spectra, Solvents, What is a Chromophore, The Effect of Conjugation, Effect of Conjugation on Alkenes, Woodward-Fieser Rules for Dienes, Carbonyl Compounds: Enones, Woodward's Rules for Enones, α, β-Unsaturated Aldehydes, Acids, and Esters, Aromatic Compounds,etc. Visible Spectra: Color in Compounds, What To Look for in an Ultraviolet Spectrum: A Practical Guide

**Unit-3: Mass spectrometric analysis: (7L)**

Principles, instrumentation and applications of mass spectrometry; Methods of generation of ions in EI, PI, CI, FD and FAB and other techniques; Detection of ions, ion analysis, ion abundance, molecular ion peak, metastable peak, isotopes, Quasi-Equilibrium Theory; Fragmentation patterns of ions; Ionization Efficiency and Ionization Cross Section; Appearance energy, Bond dissociation energies and heats of formation; Tandem mass spectrometry; Applications of mass spectrometry to simple structural and mechanistic problems.

**Unit 4: IR Spectroscopy for Structural and Functional Group Analysis: (6L)**

The Infrared Absorption Process, Uses of the Infrared Spectrum, The Modes of Stretching and Bending, Bond properties and Absorption trends, Preparation of samples for infrared spectroscopy, What to look for when examining infrared spectra, Correlation Charts and Tables, Analysis of a spectrum for structural information: Hydrocarbon, Aromatic rings, Alcohols and phenols, Carbonyl compounds and carboxylic acid derivatives, Factors that Influence the C=O Stretching Vibration, Ethers, Sulphur and phosphorus containing compounds, Alkyl and Aryl Halides, Structure determination.

**Unit 5: Case Studies and Emerging Trends: (4L)**

Forensic applications, Quality control in pharmaceuticals, Environmental pollutant monitoring, Biospectroscopy and point-of-care diagnostics, Atmospheric measurement, Spectral database, Astrochemical measurement, and spectroscopy in space

**Reference books:**


5. Pavia, D. L., Lampman, G. M., Kriz, G. S., & Vyvyan, J. R. (2009). *Introduction to spectroscopy* (4th ed). Brooks/Cole, Cengage Learning.
6. Ellis, A. M., Fehér, M., & Wright, T. G. (2005). Electronic and photoelectron spectroscopy: Fundamentals and case studies. Cambridge University Press.

7. Kemp, W. (1991). Organic Spectroscopy. Macmillan Education UK
8. Gross, J. H. (2004). *Mass spectrometry: A textbook*. Springer.

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|---|---|---|---|---|---|
| CHM527 | **Advance Spectroscopy Lab.** | 0 | 0 | 2 | 2 |

Lab content

1. Determination of isosbestic point of indicators
2. Determination of phosphate content in soft drinks
3. Determination of iron content in a given lentil sample
4. Determination of toxic elements in packaged food items
5. Determination of Pb/Fe/Cu in a given solution by AAS

Reference books:

1. Analytical Chemistry, G. D.Christian, Wiley-Interscience

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| CHM533 | **Advanced synthetic lab.** | 0 | 0 | 2 | 2 |

1. Synthesis of Potassium Trisoxalato Ferrate and it's photochemical properties
2. Synthesis pyridyl tetrazine derivatives and their photochemistry
3. Synthesis of different Schiff base compounds and their complex formation with the 1$^{st}$ row transition elements
4. Synthesis of Aspirin and Paracetamol
5. Synthesis of calixarenes and resorcarenes.
6. Synthesis of macrocyclic compounds

Reference books:

1. Supramolecular Chemistry, J. M. Lehn, Wiley-Inter Science
2. Das, S.C. Advanced Practical Chemistry, Sixth edition,
3. An introduction to Supramolecular Chemistry, A. K. Das, CBS Publisher