IISER BERHAMPUR

BS-MS SYLLABUS

Chemical Sciences

I Semester

Course No.	Course Name	Lec Hr	Lab Hr	Tut Hr	SS Hr	Credit
BIO 101	Introduction to Biological Sciences	3	0	1	6	3
BIO 103	General Biology Laboratory I	0	3	0	0	1
CHM 101	General Chemistry	3	0	1	6	3
CHM 103	General Chemistry Laboratory	0	3	0	0	1
CDS 101	Introduction to Computers	2	1	0	6	3
HSS 103	Basics of Communication Skills	1	0	0	2	1
MTH 101	Introduction to Mathematics	3	0	1	6	3
PHY 101	Mechanics	3	0	1	6	3
PHY 103	Mathematical Methods	1	0	1	0	1
EES 101	Introduction to Earth System Sciences	3	0	1	6	3
Total		**19**	**07**	**06**	**38**	**22**

II Semester

Course No.	Course Name	Lec Hr	Lab Hr	Tut Hr	SS Hr	Credit
BIO 102	Biochemical and Cellular basis of life	3	0	1	6	3
BIO 104	General Biology Laboratory II	0	3	0	0	1
CHM 102	Basic Inorganic Chemistry	3	0	1	6	3
CHM 104	Inorganic Chemistry Laboratory I	0	3	0	0	1
HSS 104	Oral and Written Communication	1	0	0	2	1
EES 102	Introduction to Environmental Sciences	3	0	1	6	3
MTH 102	Calculus of One Variable	3	0	1	6	3
PHY 102	Electromagnetism	3	0	1	6	3
PHY 104	General Physics Laboratory I	0	3	0	0	1
Total		**16**	**09**	**05**	**32**	**19**

III Semester

Course No.	Course Name	Lec Hr	Lab Hr	Tut Hr	SS Hr	Credit
BIO 201	Introduction to Genetics and Evolution	3	0	1	6	3
BIO 203	General Biology Laboratory III	0	3	0	0	1
CHM 211	Basic Organic Chemistry	3	0	1	6	3
CHM 213	Organic Chemistry Laboratory I	0	3	0	0	1
EES 201	Foundation of Earth Sciences: Part 1 (Introduction to Mineralogy, Petrology)	3	0	1	6	3
HSS 209	Technical Writing	2	0	0	4	2
MTH 201	Linear Algebra	3	0	1	6	3
PHY 201	Waves and Introductory Optics	3	0	1	6	3
PHY 203	General Physics Laboratory II	0	3	0	0	1
Total		**17**	**09**	**05**	**34**	**20**

IV Semester

Course No.	Course Name	Lec Hr	Lab Hr	Tut Hr	SS Hr	Credit
BIO 202	Molecular Biology and Developmental Biology	3	0	1	6	3
BIO 204	General Biology Laboratory IV	0	3	0	0	1
CHM 222	Classical Thermodynamics	3	0	1	6	3
CHM 224	Physical Chemistry Laboratory I	0	3	0	0	1
EES 202	Foundation of Earth Sciences: Part 2 (Introduction to Rock Deformation and Plate Tectonics)	3	0	1	6	3
HSS 207	Macroeconomics	1	0	0	2	1
MTH 202	Multivariable Calculus	3	0	1	6	3
PHY 202	Quantum Physics	3	0	1	6	3
PHY 204	General PHY Lab III	0	3	0	0	1
CDS 202	Information for Science and Technology	2	0	0	4	2
Total		**18**	**09**	**05**	**36**	**21**

V Semester

Course No.	Course Name	Lec Hr	Lab Hr	Tut Hr	SS Hr	Credit
CHM 301	Symmetry and Group Theory	3	0	0	9	4
CHM 311	Organic Chemistry I	3	0	0	9	4
CHM 313	Organic Chemistry Laboratory II	0	6	0	3	3
CHM 321	Physical Chemistry of Solutions	3	0	0	9	4
CHM ***	Departmental Elective I	3				3/4
*** ***	Open Elective I	3				3/4
Total		**15**				**21/23**

VI Semester

Course No.	Course Name	Lec Hr	Lab Hr	Tut Hr	SS Hr	Credit
CHM 302	Chemistry of Transition Metals	3	0	0	9	4
CHM 304	Inorganic Chemistry Laboratory II	0	6	0	3	3
CHM 312	Organic Chemistry II	3	0	0	9	4
CHM 322	Principles of Quantum Chemistry	3	0	0	9	4
CHM ***	Departmental Elective II	3				3/4
*** ***	Open Elective II	3				3/4
Total		**15**				**21/23**

VII Semester

Course No.	Course Name	Lec Hr	Lab Hr	Tut Hr	SS Hr	Credit
CHM 401	Non-transition Metal Chemistry	3	0	0	9	4
CHM 411	Physical Organic Chemistry	3	0	0	9	4
CHM 421	Statistical Mechanics	3	0	0	9	4
CHM 423	Physical Chemistry Laboratory II	0	6	0	3	3
CHM ***	Departmental Elective III	3				3/4
*** ***	Open Elective III	3				3/4
Total		**15**				**21/23**

VIII Semester

Course No.	Course Name	Lec Hr	Lab Hr	Tut Hr	SS Hr	Credit
CHM 402	Applications of Modern Physical Methods	3	0	0	9	4
CHM 422	Molecular Spectroscopy	3	0	0	9	4
CHM 416	Spectroscopy and Its Application in Organic Molecules	3	0	0	9	4
CHM ***	Departmental Elective IV	3				3/4
CHM ***	Departmental Elective V	3				3/4
*** ***	Open Elective IV	3				3/4
Total		**18**				**21/24**

IX Semester

Course No.	Course Name	Lec Hr	Lab Hr	Tut Hr	SS Hr	Credit
CHM 501	Project Work					10
CHM ***	Departmental Elective V/Research Credit	3	0	0	9	4
CHM ***	Departmental Elective VI/Research Credit	3	0	0	9	4
HSS 503	Law Relating to Intellectual Property and Patents	1	0	0	2	1
Total		**1**				**19**

X Semester

Course No.	Course Name	Lec Hr	Lab Hr	Tut Hr	SS Hr	Credit
CHM 501	Project Work					18
HSS 504	Law Relating to Intellectual Property and Patents	1	0	0	2	1
Total		**1**				**19**

BS-MS SYLLABUS, CHEMICAL SCIENCE

CHM 101: General Chemistry (3)

***Learning Objectives*:**

This is an introductory course that covers fundamental concepts in general chemistry. The course will focus on a conceptual understanding of the principles of chemistry. Topics of discussion will include atomic structure, periodicity of elemental properties, chemical bonding and reactivity, electronic effects in organic molecules and properties of gases.

***Course Contents*:**

Atomic Structure, Periodic Table and the Concept of Periodicity: Atomic structure; Vector model of atom and electronic configuration of polyelectronic atoms; Atomic structure as the basis for periodicity; Applications of the periodic law. Effective nuclear charge; Slater's rules, screening effect. Size of atoms and ions, ionization energies; electronegativity, electron affinity; periodic properties of elements and periodic trends, diagonal relationships; Fajan's rules.

Chemical Bonding: Lewis theory; Formal charges, resonance and rationalization of structures; VSEPR theory and shapes of molecules. Applications of VSEPR theory in predicting trends in bond lengths and bond angles. Molecular orbital theory of homo and heterodiatomic molecules, concept of HOMO, LUMO and SOMO. The solid state structures, lattice energy and Born-Haber cycle.

Electronic effects: Dipole moment, inductive and field effects, polarizability, resonance effect, hyper-conjugation; fundamental aspects of aromaticity.

Acids and Bases: Various theories of Acids and bases; Brønsted acids and bases. Protonic acids, gas-phase *vs* solution behavior of acids. Lewis acidity, 'Hard' and 'Soft' Acids and Bases. Solid acids. Concepts of pH, pK_a, pK_b as applied in different chemical structures.

Properties of the Gaseous State: Gas Laws, equation of states, critical constants, law of corresponding states, Distribution of molecular speeds and its applications, mean-free path, compressibility factor, barometric distribution law.

Heat capacity of gases, real gases and virial expansions.

***Suggested Books*:**

- *Concise Inorganic Chemistry*, J. D. Lee, Fifth Edition, Blackwell Publishing, 2006.
- *Basic Inorganic Chemistry*, F. A. Cotton, G. Wilkinson, P. L. Gaus, Third Edition, John Wiley and Sons Press, 1995.
- Shriver and Atkins, *Inorgranic Chemistry*, Ed. 4th, Oxford University Press 2006.
- Atkins, P.W., de Paula, J., *Physical Chemistry*, Ed. 9th, Oxford University Press 2009.
- *Chemistry and Chemical Reactivity,* J. C. Kotz, P. M. Treichel, J. R. Townsend, *7th Edition, Brooks/Cole, Cengage Learning, Canada,* 2010.
- *Chemistry*, R. Chang, 9th edition, McGraw-Hill, 2006.

CHM 102: Basic Inorganic Chemistry (3)

Prerequisites (Desirable): *CHM 101, CHM 103*

***Learning Objectives*:**

The concepts related to a fundamental understanding of inorganic chemistry, namely bonding, structure and reactivity shall be covered in this course.

***Course Contents*:**

Concepts and principles of non transition metal chemistry: An overview of bonding models in inorganic chemistry, Chemical forces, Bent's rule, Application of molecular orbital theory to polyatomic molecules (localized and delocalized orbitals), Walsh diagrams.

Main group Chemistry: General characteristics of s- and p-block elements [hydrides, oxides, halides], comparative study of second short period elements (B to F) with heavy congeners (Al to Cl). Electron deficient molecules, hyper-valency, concept of multi-centered bonding.

Oxidation and Reduction: The central role of transfer of electrons in chemical processes. The importance of splitting of water. Redox chemistry of extraction (Ellingham diagrams). Conversion of chemical energy into electricity. Batteries and modern state of solid state batteries, Fuel cells.

Transition metal complexes: General characteristics of transition metals and variable oxidation states. Types of ligands and stereochemistry of complexes. Preliminary idea about crystal field theory [CFT] (splitting of d-orbital energy levels for O_h, T_d and square planar complexes), application of CFT to explain color and magnetism of transition metal complexes. Concept of 18 electron rule among transition metal complexes. Preliminary ideas about relationship of transition metal complexes and metalloenzymes.

Radioactivity and Nuclear Chemistry: The nature of radioactive radiations, detection and measurements. Theory of disintegration, disintegration series. Half-life and average life period, artificial radioactivity, applications. Nuclear fission, nuclear fusion, critical mass.

Analytical Chemistry: Errors in Chemical Analysis, Precision and Accuracy, Mean, Median, Range, Standard deviation in measurements.

***Suggested Books*:**

- *Inorganic Chemistry*, Shriver and Atkins, Fourth Edition, Oxford University Press, 2006.
- *Concise Inorganic Chemistry*, J. D. Lee, Fifth Edition, Blackwell Publishing, 2006.
- *Basic Inorganic Chemistry*, F. A. Cotton, G. Wilkinson, P. L. Gaus, Third Edition, John Wiley and Sons Press, 1995.
- *Concepts and Models of Inorganic Chemistry,* B. Douglas, D. McDaniel, J. Alexander, Wiley India (P.) Ltd., India,2010.

CHM 103: General Chemistry Laboratory (1)

***Learning Objectives*:**

To learn practical experimental execution of basic chemical reactions including synthesis, purification, analysis, kinetics etc.

Suggested Experiments:

- Synthesis of cyclohexanone oxime.
- Acetylation of salicylic acid.
- Synthesis of polymer, Nylon 6-10.
- Determination of strength of acid and base.
- Estimation of acetic acid in vinegar solution.
- Preparation of hexamine nickel chloride $[Ni(NH_3)_6]Cl_2$.
- Detection of common cations and anions.
- The clock reaction
- Thin Layer Chromatography
- Photochemical reduction of ferric oxalate.

CHM 104: Inorganic Chemistry Laboratory I (1)

Suggested Experiments:

- Estimation of Calcium in Milk Powder through EDTA complexometry.
- Estimation of Iodine in Iodized common salt.
- Determination of Acid neutralizing power of Commercial Antacids.
- Estimation of Phosphoric acid in a Cola by Mo-Blue method.
- Recycling of Aluminum: Preparation of Potash Alum from waste Aluminum
- Blueprinting: Study of Photochemical Reduction of a Ferric salt.
- Preparation of $[Ni(NH_3)_6]^{2+}$&Ni estimation (Complexometry & Gravimetrically)
- Caffeine Isolation from Tea Leaves.
- An Experiment of Chromatography: Both TLC and Column separations.
- Separation of b-Carotene & Chlorophyll from Spinach extract by Paper Chromatography
- Preparation of Ni or Co-Acetylacetonate.
- Preparation of a Metal Complex with a Multidentate Ligand: Preparation of Poly-nuclear Thiourea Complex of Copper (I)
- Preparation of a Polystyrene Film.

CHM 211: Basic Organic Chemistry (3)

***Learning Objectives*:**

This is a course in basic organic chemistry that aims to provide a general understanding of organic chemistry. The initial classes will include discussion of structure, conformation and stereochemistry of organic compounds. Later, fundamental principles of organic reactions will be developed through understanding of reactivity of the important functional groups in organic compounds, reactive intermediates and molecular rearrangements.

***Course Contents*:**

Stereochemistry:

Fischer, Newman, saw-horse, etc., projection formulae

Conformational analysis of ethane, propane, butane, cyclohexane and monosaccharides

Stereoisomerism, configuration (*R*, *S*), optical isomerism in compounds with one and two chiral centers, and without an asymmetric atom, nomenclatures such as erythro, threo, *α*, *β*, endo, exo epimers, anomers, *E*, *Z*, etc., resolution of racemic compounds

Biodiscrimination of stereoisomers (amino acids, thalidomide, DOPA, nicotine, morphine)

Reactive Intermediates and molecular rearrangements:

Introduction to structure, formation, stability and reactions of carbocations, carbanions, free radicals, radical anions, radical cations, arynes, carbenes and nitrenes (in brief)

Molecular rearrangements (basic principles and migratory aptitude): Wolff, Curtius, Beckmann, Baeyer-Villiger, pinacol-pinacolone, etc.

Organic Reactions:

Electrophilic and radical additions to alkenes, electrophilic and nucleophilic aromatic substitutions, nucleophilic aliphatic substitutions: S_N1, S_N2, S_Ni reactions, neighbouring group participation, elimination reactions: E1, E2, and E1cB reactions

Functional group transformations and their reaction mechanisms

***Suggested Books*:**

- Clayden, J., Greeves, N., Warren, S., Wothers, S. *Organic Chemistry*, Oxford University Press, **2001**.
- Hornback, J. M. *Organic Chemistry*, Cengage Learning, **2006**.
- Solomons, T. W. G., Fryhle, C. B. *Organic Chemistry*, John Wiley and Sons, **2007**.
- Morrison, R. M., Boyd, R. N. *Organic Chemistry*, Pearson Education, **2008**.
- Sykes, P. A. *A guide book to mechanism in organic chemistry*, Longman, **2008**.

CHM 213: Organic Chemistry Laboratory I (1)

***Learning Objectives*:**

This is a basic organic chemistry practical course. In this laboratory course, students would be able to use their knowledge of chemical reactivity to plan and execute the preparation of compounds using various C-C and C-hetero bond-forming reactions and various organic transformations from commercially available starting materials. Upon completion of this laboratory course, the students would also get confidence on working independently and characterize the synthesized compounds using various modern techniques.

Suggested Experiments:

- Calibration of melting point apparatus thermometer
- Hydrolysis of ester: Preparation of salicylic acid from methyl salicylate
- Etherification of alcohol: Preparation of 2-ethoxynaphthalene
- Preparation of amide: Synthesis of acetanilide from aniline
- Oxidation of olefin with $KMnO_4$: Preparation of adipic acid from cyclohexene
- Reduction of ketone: Preparation of benzhydrol by $NaBH_4$ reduction of benzophenone
- Aldol reaction: Preparation of dibenzylideneacetone
- Electrophilic aromatic substitution: Nitration of acetanilide
- Nucleophilic substitution reactions: The effect of substrate structure on the reactivity under S_N1 and S_N2 conditions
- Preparation of pyridinium chlorochromate (PCC)
- Beckmann rearrangement: Preparation of benzanilide from benzophenone oxime
- Esterification of an aromatic acid.
- Synthesis of an azo-dye.
- Dakin oxidation of an aromatic aldehyde.

CHM 222: Classical Thermodynamics (3)

Zeroth law of thermodynamics and concept of temperature. First Law of thermodynamics, second law of thermodynamics and concept of entropy, free energy, criteria for equilibrium and stability, third law of thermodynamics.

Phase rule, Claussius-Clayperon equation, phase transitions in one-component systems, chemical equilibrium, interrelations between K_p, K_c and K_x, effect of temperature and pressure on equilibrium constant.

Ideal and non-ideal solutions. Raoult's law and Henry's law. Colligative properties.

***Suggested Books*:**

- Atkins, P.W., de Paula, J., Physical Chemistry, Ed. 9th, Oxford Press, **2009**.
- Levine, I., Physical Chemistry, Ed. 6th, McGraw Hill, **2009.**
- Berry, R.S., Rice, S.A., Ross, J., Physical Chemistry, Ed. 2nd, Oxford Press, **2000**.
- Castellan, G.W., Physicsl Chemistry, Ed. 3rd, Narosa Publishing House, **2004**.

CHM 224: Physical Chemistry Laboratory I (1)

Suggested Experiments:

- Determination of acid dissociation constant (pKa) of (A) polybasic acid (H_3PO_4) (B) Monobasic Acid (CH_3COOH)
- Acidic and basic dissociation constants of glycine and its isoelectronic point
- Determination of dissociation constant and equivalent conductance at infinite dilution of weak electrolyte (acetic acid) using conductometry
- Kinetics of saponification of ethyl acetate using conductometry
- Kinetics of the iodide-hydrogen peroxide clock reaction
- Potentiometric Titration of a standard solution of KCl against $AgNO_3$ – Determination of solubility product of AgCl
- Potentiometric Titration of a standard solution of $AgNO_3$ against mixture of halides – Determination of concentration of two salts in a given mixture
- First order kinetics – Acid hydrolysis of methyl acetate (at 30°C) taking different concentrations of [H+] ions.
- First order kinetics – Acid hydrolysis of methyl acetate (at 40°C) taking different concentrations of [H+] ions.

CHM 301: Symmetry and Group Theory (4)

Prerequisites: *CHM 102*

***Learning Objectives*:**

To learn the basic concepts related to symmetry elements, symmetry operations, point groups and their applications towards the understanding of bonding and spectroscopic characterization in molecules.

***Course Contents*:**

*Molecular Symmetry**:*** Symmetry elements and symmetry operations, definition of group and its characteristics, subgroups, classes, similarity transformation. Products of symmetry operations, relations between symmetry elements and operations, symmetry elements and optical activity, classes of symmetry operations, Conventions regarding coordinate system and axes, point group and classification, degenerate point groups, examples, Some properties of matrices, representation of groups, reducible and irreducible representations, the great orthogonality theorem, character tables, position vector and base vector as basis for representation, Wave functions as basis for irreducible representations (p- and d-orbitals) direct product, vanishing integral.

Symmetry adopted linear combinations: Projection operators and some examples, e.g. π-orbitals for the cyclopropenyl group etc.

Applications:

Symmetry Aspects of Molecular Orbital Theory: General Principles, symmetry factoring of secular equations, carbocyclic systems, more general cases of LCAO-MO bonding, examples, Huckel Molecular orbital theory systems, e.g., π-systems and conjugated π-systems, benzene and naphthalene, delocalization energies, resonance energies and aromaticity, the bond order (p) and free valence number (F), three centre bonding.

Hybrid orbitals and Molecular orbitals: transformation properties of atomic orbitals, hybridization schemes for bonding and for π -bonding, hybrid orbitals as LCAO, examples, MO theory for AB_n, molecular orbital theory for regular octahedral and tetrahedral molecules.

Molecular Vibrations: Normal Mode analyses *via* IR and Raman spectroscopy. Selection rules, spectral transition probability, vibronic coupling, electronic spectra of inorganic complexes and ions. Splitting of one electron level in an octahedral and tetrahedral environment.

***Suggested Books*:**

- *Chemical Applications of Group Theory*, F. A. Cotton, 3rd edition, Wiley InterScience, New York, **1990**.
- *Molecular Symmetry and Group Theory*, R. L. Carter, John Wiley & Sons, India, **2004**, **2005**.
- *Molecular Symmetry and Group Theory*, A. Vincent, 2nd Edition, John Wiley & Sons Ltd, England, **2001**.
- *Symmetry and Spectroscopy of Molecules*, K. Veera Reddy, New Age International (P) Ltd, India, **2010**.
- *Group Theory and Chemistry*, D. M. Bishop, Dover Publications, New York, **1993**.

CHM 302: Chemistry of Transition Metals (4)

Prerequisites: *CHM 102, CHM 301*

Coordination Chemistry: Coordination number and stereochemistry of coordination complexes (coordination number 2-9). Electronic configurations and states, the group state and energy levels, free-ion term, Symmetry orbitals and bonding in transition-metals complexes: L-S coupling for d_n states, splitting of one electron levels in an octahedral and tetrahedral environment, Orgel and Tanabe-Sugano diagrams, Charge-Transfer bands, Jahn-Teller distortion. Applications of CFSE, Stereochemistry of non-rigid and fluxional molecules. Thermodynamic aspects of coordination complexes, Nephelauxetic effect, Irving William series, Factors affecting ligand field stabilization energies, First row transition elements, heavy transition elements, M-M bonded complexes, C-H activation, agostic interactions, ortho-metallation. Kinetic aspects: reaction and aquation rates, electron transfer reactions. Reaction mechanism in inorganic reactions. Redox reactions, Trans effect.

*Chemistry of Lanthanides and Actinides**:*** Electronic configuration, colour and magnetism, properties of lanthanides and actinides. Synthesis of trans-Uranic elements, chemistry of uranium compounds.

Organometallic chemistry: 18e rule and its exceptions, isolobal and isoelectronic analogies. s and π bonding, types of ligands, soft *vs* hard ligands. Structure, bonding and reactivity studies of metal carbonyls, nitrosyls, dinitrogen complexes. Homogeneous and heterogeneous catalysis, oxidative addition, reductive elimination reactions, organometallic complexes with metal-metal bonds.

*Molecular Magnetism**:*** Paramagnetism, Diamagnetism and Ferromagnetism, Neel and Curie Temperature, Magnetic Susceptibility.

Inorganic Chemistry of Biological Systems: Essential and trace elements in biological systems, energy sources for life, metalloporphyrins, dioxygen binding, transport, and utilization.

***Suggested Books*:**

- Inorganic Chemistry-Principles of Structure and Reactivity. J. E. Huheey, E. A. Keiter, R. L. Keiter, 4th Edn. Harper-Collins, NY, **1993**.
- Chemistry of the Elements. N. N. Greenwood, and Earnshaw, A. 1st Edn. Pergamon, Oxford, **1989**.
- Concepts and Models of Inorganic Chemistry. B. Douglas, D. McDaniel, J. Alexander, 3rd Edn. John Wiley, New York, **1993**.
- Advanced Inorganic Chemistry. F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, 3rd Edn. John Wiley and Sons Press, **1995**.
- Modern Inorganic Chemistry. W. L. Jolly, 2nd Edn. McGraw-Hill, NY, **1991**.
- Inorganic Chemistry. D. F. Shriver, and P. W. Atkins. 3rd Edn. Oxford University, Oxford, **1999**.
- Theoretical Inorganic Chemistry, M. C. Day, 2nd Edition, East-West Press, India, **2007**.
- Essential Trends in Inorganic Chemistry, D. M. P. Mingos, OUP, New York **2010**.
- Inorganic Chemistry, G.Wulfsberg, Viva Books P. Ltd, India, **2010**.
- *Advanced Structural Inorganic Chemistry,* W.-K. Li, G.-D. Zhou,T. C. W. Mak, IUCr Monograph, OUP, New York, **2008**.

CHM 304: Inorganic Chemistry Laboratory (3)

Prerequisites: *CHM 101, CHM 102, CHM 103, CHM 104, CHM 213*

Suggested Experiments:

- Determination of spectrochemical order of ligands by using electronic spectroscopy of Nickel(II) coordination complexes.
- Demonstration of *cis-trans* isomerisation in coordination chemistry: Case of Cobalt(III) complexes
- Chemistry of a five-coordinate d^1 complex: Case of $V(O)(acac)_2$.
- The effect of symmetry on the infrared spectrum of the sulphate group
- Synthesis and catalytic application of a solid acid, 12-Tungstosilicic acid.
- Synthesis, purification, and metallation of a bio-inorganically important porphyrin ligand
- Organometallic synthesis: Synthesis of ferrocene
- NMR spectroscopic investigation of molecular fluxionality: Case of an allyl-palladium complex
- Synthesis and electrochemistry of $[Ru(bpy)_3]^{2+}$.
- Preparation, recording and indexing of PXRD patterns of simple cubic solids.
- Synthesis of 123-superconductor.

CHM 311: Organic Chemistry I (4)

Prerequisites: *CHM 101, CHM 211*

***Learning Objectives*:**

This is a fundamental course where student initially can learn stereochemistry of organic molecules such as conformational analysis of cyclic and acyclic compounds. Further, dynamic stereochemistry and reactivity of simple molecules will be discussed. In the second part, various rearrangement (electrophillic, nucleophillic, sigmatropic, etc) reactions would be covered. In the third part of this course, the functional group inter-conversion based on oxidation and reduction protocols would be covered.

***Course Contents*:**

Stereochemistry:

- Conformational analysis, conformation of acyclic, cyclic, fused and bridged systems
- Strain in cyclic and acyclic molecules including allylic strain (A1,2 and A1,3)
- Dynamic stereochemistry: Conformation and reactivity, Curtin-Hammett principle

Rearrangement Reactions:

- Electrophilic (Beckmann, Hofmann, Lossen, Curtius, Wolff, Schmidt, Baeyer-Villiger, Pinacol-pinacolone, Wagner-Meerwein etc.), nucleophilic (benzilic acid, Favorskii), and radical rearrangements (Wittig, aza-Wittig)
- Sigmatropic rearrangements (Cope, aza-Cope, Oxy-Cope, Claisen, aza-Claisen, Eschenmoser-Claisen, vinyl cyclopropane-cyclopentene)
- Miscellaneous (Brook, Pummerer)

Oxidations:

- Oxidation of alcohols, ketones and aldehydes (transition metal oxidants, hypervalent iodine based, sulphur based, peroxide and peracid, etc.)
- Oxidation of C-C double bonds (Ozone, $KMnO_4$, $Pb(OAc)_4$, Dimethyldioxirane, OsO_4, 2-sulfonyl oxaziridine etc.)
- Oxidation at unfunctionalized carbon

Reductions:

- Reduction of carbonyl compounds (hydrogenation, reductions using group III, IV hydride donors, reductive deoxygenation), carbon-carbon multiple bonds (catalytic hydrogenation, diimide reduction) and other selected functional groups
- Dissolving metal reductions

Heterocyclic Chemistry:

- General overview and nomenclature of heterocyclic compounds (structure of 3 to 7 membered saturated and 5,6 membered aromatic heterocycles)
- Synthesis and reactions of heterocyclic compounds (in brief)

***Suggested Books*:**

- Clayden, J., Greeves, N., Warren, S., Wothers, S. *Organic Chemistry*, Oxford University Press, **2001**.
- Eliel, E. L., Wilen, S. H., Doyle, M. P. *Basic Organic Stereochemistry*, John Wiley and Sons, **2001**.
- Smith, M. B. and March, J. *Advanced Organic Chemistry*, Wiley Interscience, **2007**.
- Carey, F. A, Sundberg, R. J. *Advanced Organic Chemistry*, *Part A and B*, Springer, **2007**.
- Anslyn, E. V., Dougherty, D. A. *Modern Physical Organic Chemistry*, University Science Books, **2005**.
- Hornback, J. M. *Organic Chemistry*, Cengage Learning, **2006**.

CHM 312: Organic Chemistry II (4)

Prerequisites: *CHM 101, CHM 211, CHM 311*

Carbon-Carbon Bond Forming Reactions:

- *via* enolate, enamine and imine chemistry
- Grignard, cuprate and other conjugate reactions
- Olefination (Wittig, HWE, Julia and Peterson) and cyclopropanation reaction
- Radical reactions
- Other classes (via organo silane, borane and tin based reagents, Baylis-Hillman reaction)
- Introduction to Pericyclic reactions

Enantioselective Reactions:

- Principles of enantioselective reactions
- Enantioselective reduction of carbonyl compounds (Corey's oxazaborolidine catalyzed reductions and Noyori's BINAP reduction)
- Enantioselective epoxidation of olefins (Sharpless, Jacobsen, Shi, etc.)

Introduction to Retrosynthesis:

- Basic concepts of retrosynthesis
- Demonstration of its utility with few examples

***Suggested Books*:**

- Clayden, J., Greeves, N., Warren, S., Wothers, S. *Organic Chemistry*, Oxford University Press, **2001**.
- Carruthers, W., Coldham, I. *Some Modern Methods of Organic Synthesis*, Cambridge University Press, **2004**.
- Smith, M. B. and March, J. *Advanced Organic Chemistry*, Wiley Interscience, **2007**.
- Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry*, *Part A and B*, Springer, **2007**.
- Smith, M. B. *Organic Synthesis*, McGraw-Hill, **2001**.
- Warren, S. *Organic Synthesis: The Disconnection Approach*, Wiley, **1983**.

CHM 313: Organic Chemistry Laboratory II (3)

Prerequisites: *CHM 213, CHM 311*

***Learning Objectives*:**

This is an advanced organic chemistry practical course. In this laboratory course, students would be able to use their knowledge of selectivity in synthesis (chemo-, regio- and stereoselectivity) to plan and execute the preparation of complex organic compounds using modern C-C and C-hetero bond-forming reactions. This course would involve multi-step synthesis and chromatographic analysis of complex mixtures and advanced characterization techniques. Upon completion of this laboratory course, a student would be confident on working in a synthesis laboratory and also be able to characterize simple compounds using various modern spectroscopic techniques.

Suggested Experiments:

- Preparation of Corey-Bakshi-Shibata (CBS) reagent and enantioselective reduction of a carbonyl compound.
- Preparation of pentacyclic dione via Diels-Alder and photochemical cyclizations.
- Preparation of a Wittig salt and olefination of a carbonyl compound
- Preparation of Evans chiral auxiliary and its use in asymmetric aldol reaction
- Preparation of a Grignard reagent and its addition to a carbonyl compound
- Generation and trapping of benzyne
- Generation of a carbene: The Reimer-Tiemann reaction
- The Fischer indole synthesis
- Sonogashira/Suzuki/Heck coupling reaction
- Olefin metathesis (using Grubbs 1st generation catalyst)
- Baylis-Hillman reaction
- Synthesis of L-Prolinamide ligands
- Synthesis of BINOL
- Synthesis of β-nitro styrene (Henry reaction)
- Ugi multicomponent coupling.

CHM 318: Photochemistry and Heterocyclic Chemistry (4)

Pre-requisites (Desirable)*: CHM 211 Basic Organic Chemistry*

Learning Objectives**:**

To understand the chemical transformations achievable through use of light and how interaction between light and organic compounds generates reactive oxygen species, produces new molecules and generate light from chemical reactions. What are the common properties of heterocyclic compounds, how they are synthesized and utilized in chemistry and biology.

Course Contents**:**

Photophysical processes (Jablonskii diagram, Internal conversion, Inter system crossing, Quantum yield); Bimolecular Photophysical Processes – Excimers, Exciplexes, Photoinduced Energy Transfer, Quenching etc. Photochemical reactions and processes, Chemiluminescence, Singlet oxygen and related reactions.

Nomenclature of heterocycles, structure and properties of common heterocycles, synthesis of Indoles, Quinolines, Isoquinolines, Furans, Pyrroles, Thiophenes etc., Typical reactivity of aromatic heterocycles, heterocycles with more than two heteroatoms, heterocycles in biological systems

Suggested Books**:**

- *Modern Physical Organic Chemistry* by E. V. Anslyn and D. A. Dougherty, University Science Books, 2006.
- *Heterocyclic Chemistry* by J. A. Joule and K. Mills, Wiley, 5th Edition, 2010

CHM 321: Physical Chemistry of Solutions (4)

Prerequisites: *CHM 222*

***Learning Objectives*:**

Concepts related to chemical kinetics, basic electrochemistry and phase equilibrium of binary mixtures will be discussed. This course is crucial for chemistry students irrespective of specialization since chemical kinetics, solution property are important for all branches of chemists.

***Course Contents*:**

Phase transitions in multi-component systems.

Ionic solutions: Mechanism of electrolysis and Faraday's laws. Conductance, electrolytic conductance, solvation of ions, Debye-Huckel-Onsager conductance equation, degree of dissociation, transport number, free energy and activity, Debye-Huckel limiting law, solubility equilibria, overview of electrode processes, electrical double layer, Faradaic reactions, mass transfer controlled reactions, coupled chemical reactions.

Electrochemistry: Electrochemical cells and reactions, basics of electrochemical thermodynamics, Nernst equation, Butler-Volmer model.

Chemical kinetics: Order and molecularity, kinetics of zero, first and second order reactions. Parallel, reversible and consecutive reactions. Concept of steady state and its application. Arrhenius equation, Lindemann hypothesis, collision rate theory, transition state theory. Enzyme kinetics and catalysis.

***Suggested Books*:**

- Atkins, P. W., de Paula, J., *Physical Chemistry*, Ed. 9th, Oxford Press, **2009.**
- *Physical Chemistry,* Gilbert W Castellan.
- *Physical Chemistry,* Ira N. Levine.
- *Chemical Kinetics*, Keith J. Laidler.
- *An Introduction to Electrochemistry,* Samuel Glasstone.
- *Electrochemical Methods: Fundamentals and Applications*, Allen J Bard and Larry R. Faulkner, 2nd Edition, John Wiley and Sons.
- *Modern Electrochemistry Ionics: Volume 2*, John O'M. Bockris and Amulya K. N. Reddy, 2nd Edition, Plenum Press.

CHM 322: Principles of Quantum Chemistry (4)

Pre-requisites *:MTH 101, PHY 101, CHM 101, MTH 102, PHY 102, MTH 201, PHY 201 or their equivalent (Not allowed for Physics majors)*

***Learning Objectives*:**

This course will give basic conceptual understanding and application of quantum mechanics to simple atomic and molecular systems, and prepare the students for learning more in-depth quantum chemistry.

***Course Contents*:**

1. **A brief review of classical mechanics**: Newton's laws of motions – kinetic energy and potential energy, conservative force. Generalized coordinates. Lagrange's equations of motions. Hamilton's equations of motions. Poisson brackets.
2. **The need for quantum mechanics**: Review of early experiments and old quantum theory: Black-body radiation, photoelectric effect, line spectra of atoms and Bohr model of hydrogen atom, Compton effect, Frank-Hertz experiment. Young's double-slit experiment and wave-particle duality. de Broglie wavelength, uncertainty principle, superposition and state of a quantum system.
3. **States in quantum mechanics**: Stern-Gerlach experiments and its different variations. States, superposition of states. Statistical nature of quantum measurements.
4. **Postulates of quantum mechanics**: States and wavefunctions, Time-dependent Schrödinger equation. Observables and the measurement hypothesis, Born's interpretation of wavefunction, time evolution of states, stationary states, time-independent Schrödinger equation. Heisenberg's equation of motion and Ehrenfest's relations.
5. **Mathematical background**: Operators in quantum mechanics and their properties, eigenvalues and eigenfunctions, commutation relations, unitary transformations and change of basis. Matrix representation of operators. Compatible observables and the generalized uncertainty principle.
6. **One-dimensional problems**: A free particle, particle in a well and transmission through a barrier. Probability currents and the equation of continuity. Two and three-dimensional potential wells and degeneracy. Applications to conjugated molecules and other one-dimensional systems. Linear harmonic oscillator – ladder operator method, parity of harmonic oscillator eigenfunctions. Rigid rotor problem, angular momentum, angular momentum eigenvalues and eigenfunctions.
7. **The hydrogen atom**: Atomic orbitals – radial and angular wavefunctions and distributions, electron-spin and spin operators. Virial theorem and application to hydrogen atom and other problems. Hydrogen-like atoms.
8. **Approximation methods**: Variation method – He atom,Time-independent perturbation theory – Anharmonic oscillator, He atom, H 2 + molecular ion. H 2 molecule and the LCAO approach. Time-dependent perturbation theory, Fermi's golden rule, transition probability and the basis of selection rules.
9. **Atoms in external fields**: Zeeman effect and Stark effect.

***Suggested Books*:**

1. Pilar, F. L., Elementary Quantum Chemistry, 2nd ed., McGraw-Hill, New York, 1990.
2. Sannigrahi, A. B., Quantum Chemistry, 2nd ed., Books & Allied, Kolkata, 2020.
3. Levine, I., Quantum Chemistry, 6th ed., Pearson Press, 2009.
4. McQuarrie, D. A., Quantum Chemistry, 2nd ed, University Science Books, 2008.

5. Pauling, L., Wilson, E. B., Introduction to Quantum Mechanics, McGraw-Hill, New York, 1935.
6. Atkins, P. W., Friedman, R. S., Molecular Quantum Mechanics, Oxford University Press, 2008.
7. Eyring, H., Walter, J., and Kimball, G. E., Quantum Chemistry, John Wiley, New York, 1944.
8. Zettili, N., Quantum Mechanics, 2nd ed., John Wiley, 2009.

CHM 323: Solid State Chemistry (4)

Prerequisites: *CHM 101, CHM 102, CHM 222*

General Concepts, Definitions: Structures of Ionic Solids (crystal chemistry), Metals and Alloys, Band Theory in Solids (Metals, Semiconductors, Inorganic Solids), crystal defects, non-stoichiometric compounds, solid solutions, dislocations and stacking faults.

Structure and Bonding in Solids (Crystalline and Amorphous): Factors governing formation of crystal structures, Lattice Energy, Effective nuclear charge, Kapustinskii's equation, Sanderson's Model, Bond Energy and Bond Order calculations, Mooser-Pearson plots, Ionicities, bond valence, bond length, non-bonding electron effects.

Phase Transitions: Buergers's (reconstructive and displacive), Ubbelohde's Classification (continuous and discontinuous), Applications of G-T diagrams, kinetics, critical size and nucleation rate, Avrami Equation, Martensitic, order-disorder transitions.

Ionic Conductivity and Solid Electrolytes: Conduction Mechanisms, Alkali Halides, Lithium, Silver, Oxide and Halide Ion conductors, Conductivity measurements (D.C. and A.C methods), Applications to electrochemical cells, batteries, sensors, and fuel cells.

Structure Property Correlation in Inorganic materials: Electronic, Electrical, Magnetic, Optical (Luminescence), Dielectric, Ferroelectric and superconductivity.

Preparative methods: Oxides, nitrides, fluorides and characterization of inorganic solids by different physical (diffraction, microscopic and spectroscopic) techniques.

***Suggested Books*:**

- Solid State Chemistry and its Applications: West, A. R. John Wiley & Sons, UK, 1987.
- Structure and Bonding in Crystalline Materials: Rohrer, G. S. 1st edition, Cambridge University Press, UK, 2001.
- New Directions in Solid State Chemistry: Rao, C. N. R. Gopalakrishnan, J. 2nd edition, Cambridge University Press, UK, 1997.

CHM 324: Physical Properties of Matter (4)

Prerequisites: *CHM 222, CHM 321*

Intermolecular forces - excluded volume, Dispersion forces, van der Waals forces, dipolar interactions, hydrogen-bonding, covalent interactions, Lennard-Jones potential and Morse potential, electrostatic interactions, multipole expansions, polarizability.

Transport properties, Surface phenomena, adsorption kinetics, Langmuir, Freundlich and BET isotherms, surface tension, capillary rise and basic applications.

Micelles and reverse micelles, colloids, thermodynamics of polymer solutions.

Collision theory and potential energy surfaces.

***Suggested Books*:**

- Atkins, P. W. and de Paula, J., *Physical Chemistry*, Ed. 9th, W. H. Freeman, **2009**.
- Silbey, R. J., Alberty, R. A., and Bawendi, M. G., *Physical Chemistry*, Ed. 4th, Wiley, **2004**.
- Berry, R. S., Rice, S. A., and Ross, J., *Physical Chemistry*, Ed. 2nd, Oxford, **2000**.

CHM 325: Mathematical Methods for Chemists (4)

Prerequisites: *MTH courses taught in first and second years.*

***Learning Objectives*:**

To provide students of chemistry with the necessary skills and confidence to apply simple ideas and methods in mathematics for solving problems in physical chemistry and quantum chemistry.

***Course Contents*:**

- **Infinite series and power series:** Infinite series and their convergence and divergence. Test of convergence – comparison test, integral test, ratio test. Absolute and conditional convergence. Power series and their region of convergence, Maclaurin series, Taylor series. Series expansion of some simple functions.
- **Linear algebra:** Matrices, determinants, addition, multiplication and inverse of matrices, vectors, linear combination, linear functions, linear operators, linear dependence and independence, special matrices – real, symmetric, anti-symmetric, Hermitian, orthogonal and unitary. Orthogonal transformations – rotations in 2 and 3 dimensions, Euler angles. Linear vector space, orthonormal basis, eigenvalues and eigenvectors of a square matrix, diagonalisation of a square matrix. Matrices and linear operators, Hermitian operators, projection operators.
- **Differential equations:** Types of differential equations with examples: ordinary differential equations (separable, first, and second order equations) & partial differential equations, Methods for solving differential equations: separation of variables, series solution of ordinary differential equations (Legendre & Bessel equations), Expansion about a regular singular point. Laplace transform and power series (Frobenius) methods of solving linear differential equations. Applications to problems in chemistry.
- **Orthogonal functions:** Even and odd functions, complete set of functions, orthogonal and orthonormal functions, expansion in terms of orthonornal functions, Fourier series, construction of orthonormal functions by Gram-Schmidt procedure, Schwarz inequality. Hermite, Legendre and Laguerre polynomials and their properties, generating functions and differential equations associated with these polynomials, recursion relations. Highlight their applications in quantum mechanics/chemistry.
- **Vector analysis:** Scalar and vector multiplications, triple products, differentiation of vectors, directional derivative, gradient, curl, successive application of the differential operator, line integrals, conservative fields, potentials, exact differentials, Green's theorem in the plane, divergence and divergence theorem, curl and Stokes' theorem.
- **Tensor analysis:** Cartesian tensors, tensor notation and operations, Kronecker delta and Levi-Civita symbol. Moment of inertia and other examples of 2nd rank tensors in molecules and materials.
- **Curvilinear coordinates:** General curvilinear coordinates, vector operators in orthogonal curvilinear coordinates, Laplacian operator in cylindrical, plane polar and spherical polar coordinates. Highlight their applications in quantum mechanics/chemistry.
- **Complex numbers:** Complex numbers as an ordered pair of numbers, as a point in a 2-dimensional space. Complex plane and Argand diagram, complex algebra, complex power series and disk of convergence, Euler's formula, powers and roots of complex numbers, exponential and trigonometric and hyperbolic functions, logarithms, complex roots and powers, inverse trigonometric and hyperbolic functions.
- **Functions of a complex variable:** Analytic functions, Cauchy-Riemann conditions, regular points and singular points, contour integrals, Cauchy's integral theorem, Cauchy's integral formula, Laurent series, residue theorem, evaluation of definite integrals by the use of residue theorem.

Integral transforms: Fourier transform, cosine-sine transforms, Fourier transform of derivatives, convolution theorem, general integral transforms, Laplace transform, convolution, Inversion formula for Laplace transform.

Suggested Readings **:**

- Boas, M. L, Mathematical methods for the physical sciences, Kaye Pace, Ed. 3rd, 2006.
- McQuarrie, D. A., Mathematical methods for scientists and engineers, University Science Books, 2003.
- Anderson, J. M., Mathematics for quantum chemistry, Dover Publications 2005.
- Riley,K. F., Hobson, M. P., Bence, S. J., Mathematical methods for physics and engineering, Cambridge University Press, 3rd Ed., 2012.
- Bell, W. W., Special functions for scientists and engineers, Dover Publications 2004.
- Arfken, G., Weber, H., and Harris, F., Mathematical methods for physicists, Academic Press, Ed. 7th, 2012.
- Kreyszig, E. Advanced engineering mathematics, 10th Ed. Wiley, 2015.

CHM 331: Fundamentals of Supramolecular Chemistry (4)

Prerequisites: *CHM 102*

Hydrogen Bonding and Nature of Supramolecular Interactions: Ion-Ion, Ion-Dipole, Dipole-Dipole, Cation-π, Anion-π, π-π, van der Waals, Close packing in Solid State and Hydrophobic Effects.

Concepts: Host-Guest Chemistry; Receptors, Coordination and the “Lock and Key” Analogy; Chelate, Conformational and Macrocyclic Effects; Pre-organisation and Complementarity; Thermodynamic and Kinetic Selectivity.

Ionic Recognition (Cation and Anion Binding Host): Selectivity and Solution Behaviour of Crown Ethers, Crytands, Spherands; Complexation of Organic Cations, siderophores, biological anion receptors, Anticrowns and Coordination Interactions.

Neutral Host Molecules: Inorganic Solid-State Clathrate compounds, clathrates of organic hosts, intracavity complexes of neutral molecules (Fullerenes and Cyclodextrins): Solution and Solid State Binding.

Crystal Engineering: Concepts of Crystal Design and Growth, Applications to Polymorphism and Cocrystal formation.

Self Assembly: Applications to Catenanes, Rotaxanes and Helicates, Role of Positive Cooperativity.

Applications: Structure and function of DNA, Supramolecular Reactivity, Liquid Crystals, Dendrimers, MOF’s, Electronic devices (switches, wires and rectifiers) and non-linear optical materials.

***Suggested Books*:**

- Supramolecular Chemistry. J. W. Steed, J. L. Atwood, John Wiley and Sons, 2000.
- Supramolecular Chemistry. Concepts and Perspectives. J. -M. Lehn. VCH, 1995.
- Principles and Methods in Supramolecular Chemistry. H.-J. Schneider, A.Yatsimirsky, John Wiley and Sons.

CHM 332: Principles of Solid State Chemistry and Crystallography (4)

Pre-requisites (Desirable)*: CHM 101, CHM 102 and CHM 301*

Learning Objectives**:**

To learn the concepts related to the arrangement of atoms in solids and how these influence the properties of matter.

Course Contents**:**

A. **Concepts**: Structures of Ionic Solids (crystal chemistry), Metals and Alloys, Band Theory in Solids (Metals, Semiconductors, Inorganic Solids), crystal defects, non-stoichiometric compounds, solid solutions, dislocations and stacking faults.
B. **Structure and Bonding in Solids**: Factors governing formation of crystal structures, Kapustinskii's equation, Sanderson's Model, Mooser-Pearson plots, non-bonding electron effects.
C. **Phase Transitions**: Buergers's (reconstructive and displacive), Ubbelohde's Classification (continuous and discontinuous), Applications of G-T diagrams, kinetics, critical size and nucleation rate, Martensitic, order disorder transitions.
D. **Structure Property Correlation in Materials**: Optical, Dielectric and Superconducting properties.
E. **Symmetry in the Solid State**: Unit Cell, Crystal Systems, Asymmetric Unit, Crystal lattices (2D), Bravais Lattices (3D), Miller planes (crystallographic directions and multiplicities) , d-spacing formula (resolution),Crystallographic Point and Space groups (equivalent points, Wyckoff positions, site occupancy factor).
F. **Elements of X-ray diffraction**: Scattering by an Atom and Crystal, Bragg's Law, Reciprocal Lattice, Reflecting and Limiting sphere of reflection, systematically absent reflections.
G. **Crystal structure determination**: Structure Factor and Phase Problem, Electron Density. Maps, Anomalous Scattering, Thermal Motion Analysis , refinement and crystallographic parameters in crystal structure analysis, dynamic and static disorder, the physical interpretation of molecular (Bond lengths, angles and torsions) and crystal structures (Packing Diagram), Rietveld method in Powder diffraction.

Suggested Books**:**

1. Solid State Chemistry and its Applications: West, A. R. John Wiley & Sons, UK, 1987.
2. Structure and Bonding in Crystalline Materials: Rohrer, G. S. 1st edition, Cambridge University Press, UK, 2001.
3. Basics of Crystallography and Diffraction: C. Hammond.
4. X-ray Structure determination: A practical guide: G. H. Stout and L. H. Jensen.

CHM 342: Macromolecular and Analytical Chemistry (4)

Prerequisites: *CHM 102*

Part A:

- Monomers, dimers, and oligomers
- Polymerization by carbonyl substitution reactions, electrophilic substitutions, S_N2 reactions, Nucleophilic attack on isocyantes
- Polymerization of olefins: radical polymerization, anionic (living polymerization) and cationic polymerization, Isotactic, Syndiotactic, and Atactic polymerization, Ziegler-Natta polymerization
- Co-polymerization: Synthetic Rubber, Cross-linking polymer
- Biodegradable polymers
- Reactions of polymers: Merrifield resins, peptide synthesis using polymer-bound reagents, polyacryl amide gels

Part B:

- Calculations used in analytical chemistry
- Errors in chemical analysis
- Classical methods of analysis: Gravimetric, Volumetric and Titrimetric, Potentiometric methods
- Separation techniques: Introduction to analytical separation, gas chromatography, and HPLC and related methods
- Preparing samples for analysis: primary, secondary standard etc.

***Suggested Books*:**

- Clayden, J., Greeves, N., Warren, S., Wothers, S. *Organic Chemistry*, Oxford University Press, **2001**.
- Skoog, West, Holler, Crouch., *Fundamentals of Analytical Chemistry*, Cengage Learning.

CHM 343: Chemistry of Biological Systems (4)

***Learning Objectives*:**

This course focuses on the Chemical aspects of Biological transformations. This course aims to introduce the chemical functionalities present in various classes of biological molecules, and discuss how transformation of these functionalities in Nature utilize the principles of Chemistry.

***Course Contents*:**

Part A:

- Carbohydrates: Monosaccharide, polysaccharides, Mutarotation, Anomeric effects.
- Amino acids and Protein structure
- Fatty acid biosynthesis and degradation pathways
- Introduction to metabolism and bioenergetics.
- Oxidation and Reduction pathways in biological system.
- Chemistry of Garlic and Onion

Part B:

- Elements of life, Role of metal ion in biological functions,
- Metal nucleic acid interactions, Metalloproteins and metalloenzymes,
- Oxygen carrier proteins- Structure and role of haemoglobin, myoglobin, hemerythrin, hemocyanin.
- Electron transport proteins: Iron-Sulfur proteins, cytochromes.
- Redox enzyme: Mo, Fe, Cu, Zn-containing redox enzyme.
- Metal induced toxicity and chelation therapy: Platinum complexes and related anticancer drugs.

***Suggested Books*:**

- Jeremy Berg, John Tymoczko, and Lubert Stryer *Biochemistry* (5th Edition)
- S. J. Lippard, J. M. Berg *Principles of Bioinorganic Chemistry* University Science Books
- Clayden, J., Greeves, N., Warren, S., Wothers, S. *Organic Chemistry*, Oxford University Press, **2001**.

CHM 401: Non-transition Metal Chemistry (4)

Prerequisites (Desirable): *CHM 102, CHM 301*

***Learning Objectives*:**

Basic understanding of the bonding concepts and principles in non-transition metal chemistry, which would be extended to explain the diverse reactivity of main group elements ranging from pure inorganic rings, clusters, polymers to well-defined organometallic compounds, and macromolecules.

***Course Contents*:**

Concepts and principles of nontransition metal chemistry: An overview of bonding models in inorganic chemistry, Application of molecular orbital theory to polyatomic molecules (localized and delocalized orbitals), Walsh diagrams, Fluxional molecules, Atomic inversion, Berry pseudorotation.

The role of *p-* and *d-* orbital participation in nonmetals, Periodicity, periodic anomalies of the nonmetals, multiple bonding in heavier main group elements, charge transfer complexes.

Representative chemistry of s- and p-blocks: alkali metals, boranes, carboranes, boron clusters, Wade's rules, metallacarboranes, boron nitride, borylene, aminoboranes, organoaluminium compounds, graphite, diamond, fullerene, grapheme, CNT, organosilicon compounds, silicates and aluminosilicates, zeolites, silylenes and R_3Si^+, Polysilanes, stability and activation of dinitrogen, phosphorus oxides, oxyacids, phosphines, anion chemistry of N, P, As and Sb, singlet and triplet oxygen, oxygen activation, chemistry of chalcogens, polychalcogenides, sulfur-nitrogen compounds, halogens, pseudohalogens, interhalogens, noble gases, CFC

Inorganic rings and polymers: Borazines, heterocyclophosphazenes, siloxanes, stannoxanes and the polymers derived from them.

Chemistry of carbenes, push-pull carbenes, stable heavier carbene analogues (Silicon, Germanium, Tin and lead): synthesis, characterisation and reactivity.

Multiple bonding in heavier main-group elements: Synthesis, structure and reactivity.

Main group organometallic chemistry: Preparation, stability aspects and reactions. Structurally diverse *π*-cyclopentadienyl complexes of the main group elements. Element-Element Addition to Alkynes (Si-Si, Ge-Ge, B-B, S-S, Se-Se, Ge-Sn, Si-B, Sn-B, S-B, Se-P, Si-S).

Interlocked macromolecules: catenanes, rotaxanes, pseudorotaxanes.

***Suggested Readings* :**

- *Inorganic Chemistry-Principles of Structure and Reactivity.* J. E. Huheey, E. A. Keiter, R. L. Keiter, *4th Edn.* Harper-Collins, NY, **1993**.
- *Chemistry of the Elements.* N. N. Greenwood, and Earnshaw, A. *1st Edn.* Pergamon, Oxford, **1989**.
- *Concepts and Models of Inorganic Chemistry.* B. Douglas, D. McDaniel, J. Alexander, *3rd Edn.* John Wiley, New York. **1993**.

- *Advanced Inorganic Chemistry.* F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, *3rd Edn.* John Wiley and Sons Press, **1995**.
- *Modern Inorganic Chemistry.* W. L. Jolly, *2nd Edn.* McGraw-Hill, NY, **1991**.
- *Inorganic Chemistry.* D. F. Shriver, and P. W. Atkins. *3rd Edn.* Oxford University, Oxford, **1999**.
- Journal articles.

CHM 402: Applications of Modern Physical Methods (4)

Prerequisites (Desirable): *CHM 301, CHM 302*

***Learning Objectives*:**

Characterization techniques are central to synthesis of inorganic molecules. This course discusses applications of multinuclear NMR, ESR, CV, and XPES which are universal tools to investigate the structure of new molecules. In addition the course also sheds light on thermal methods namely DSC and TGA which are widely used to characterize the thermodynamic properties of solids.

***Course Contents*:**

Nuclear Magnetic Resonance Spectroscopy: Introduction, multinuclear NMR of various inorganic and organometallic compounds. [15]

Electron Paramagnetic Resonance Spectroscopy: Theory, Analysis of EPR spectra of systems in liquid phase, radicals containing single and multiple set of protons, triplet ground states. Transition metal ions, rare earth ions, ions in solid state. Double resonance techniques: ENDOR in liquid solution, powders and in non-oriented solids. [10]

Mossbauer Spectroscopy: Physical concepts, spectral line shape, isomer shift, quadrupole splitting, magnetic hyperfine interaction. Interpretation of Mossbauer parameters of ^{57}Fe and ^{119}Sn. Applications to Solid-state reactions, thermal decomposition, ligand exchange, electron transfer and isomerism. [5]

Electrochemical Methods: Heterogeneous electron transfer and concept of capacitative and Faradic current. CV, DPV and coulometry. Applications of CV in organic and inorganic chemistry. [4]

Mass Spectroscopy: Introduction and Applications to Isotopic systems. [1]

X Ray Photoelectron spectroscopy: Principles, Core level PES, Valence-electron PES, and Valence excitation spectroscopy. [4]

Thermal methods of characterization: DSC and TGA. [2]

***Suggested Readings* :**

- *NMR Spectroscopy – An Introduction*, H. Gunther, John Wiley, **1980**.
- *Inorganic Spectroscopic Methods, Alan K. Brisdon, OUP,* **2005**.
- *NMR Spectroscopy in Inorganic Chemistry,* Jonathan A.Iggo, *OUP*, **2011**.
- *NMR, NQR, EPR and Mossbauer spectroscopy in Inorganic Chemistry, R.V.Parrish, Ellis Horwood Limited, UK,* **1990**.
- *R.S.Drago Physical Methods in Inorganic Chemistry,* East-West Press Pvt. Ltd.-New Delhi,2012.
- *Structural Methods in Inorganic Chemistry*, E. A. V. Ebsworth, D. W. H. Rankin & S. Cradock, 2nd Ed.**1991**, CRC Press, Boca Raton, Florida.
- *Electrochemical methods – Fundamentals and applications*, A. J. Baird and L. R. Faulkner, Wiley, **1980**.
- *Applications of Physical Methods to Inorganic and Bioinorganic Chemistry*, R. A. Scott, C. M. Lukehart, Wiley, **2007**.

CHM 411: Physical Organic Chemistry (4)

Prerequisites: *CHM 311, CHM 312*

***Learning Objectives*:**

This course gives an in-depth understanding of a broad range of organic reactions from physical organic chemistry perspective. The topics include thermodynamic & kinetic control of organic reactions, Curtin-Hammett Principle, probing the reaction mechanisms by kinetic isotope effects, stereoelectronic effects in conformations, allylic strain and various selected reactions. Also, a detailed study and application of the theories/rules governing various pericyclic reactions will be carried.

***Course Contents*:**

Chemical Equilibria and Chemical Reactivity:

- Thermodynamic and kinetic control of reactions
- Correlation of reactivity with structure, linear free energy relationships, Hammond's postulate, Curtin-Hammett principle, substituent constants and reaction constants

Chemical Kinetics and Isotope Effects:

- Various types of catalysis and isotope effects, importance in the elucidation of organic reaction mechanisms

Stereoelectronic Effects in Organic Chemistry:

- Role of stereoelectronic effects in the reactivity of acetals, esters, amides and related functional groups
- Reactions at sp^3, sp^2, and sp carbons, Cram, Felkin-Ahn, Zimmerman-Traxler, Houk, Cieplak, exterior frontier orbital extension (EFOE) and cation-complexation models as applied to p-facial stereoselectivity
- Allylic strain ($A^{1,2}$ and $A^{1,3}$) and other strains

Pericyclic Reactions:

- Conservation of orbital symmetry, Woodward-Hoffmann rules, frontier molecular orbital (FMO) theory
- Orbital overlap effects in cycloadditions, electrocyclizations, sigmatropic rearrangements and chelotropic reactions
- Paterno-Buchi, Norrish type I and II reactions

***Suggested Readings* :**

- Isaacs, N. S. *Physical Organic Chemistry*, Prentice Hall, **1996**.
- Deslongchamps, P. *Stereolectronic Effects in Organic Chemistry*, Elsevier Science, **1983**.
- Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry*, *Part A and B*, Springer, **2007**.
- Turro, N. J. *Modern Molecular Photochemistry*, University Science Books, **1991**.
- Anslyn, E. V., Dougherty, D. A. *Modern Physical Organic Chemistry*, University Science Books, **2005**.

- Woodward, R. B., Hoffmann, R. *The Conservation of Orbital Symmetry*, Verlag Chemie, **1970**.
- Lehr, R. E., Marchand, A. P. *Orbital Symmetry: A Problem Solving Approach*, Academic Press, **1972**.

CHM 416: Spectroscopy and its Application to Organic Molecules (4)

Prerequisites: *CHM 311, CHM 312*

Infrared spectroscopy: Theory of IR spectroscopy, Modes of stretching and bending, Fourier Transform Spectrometers, Background spectrum, Survey of important functional groups with examples, Chemical environment and chemical shift.

Nuclear Magnetic Resonance: Physical basis of Nuclear Magnetic Resonance spectroscopy, Chemical shift and Spin-spin coupling as functions of structure, Analysis of high-resolution NMR spectra, FT and pulse-NMR, NOE, 2D NMR (COSY, INADEQUATE, HMQC, HSQC, HMBC, NOESY, HETCOR, ROESY, TOCSY).

Mass spectroscopy: Principles of Mass Spectrometry, Ion sources (EI, CI, Field Ionization, FAB, Plasma desorption, Field desorption, Laser desorption, MALDI, Thermospray, API, ESI, APCI, APPI, Atmospheric pressure secondary ion mass spectrometry, inorganic ionization techniques, formation and fragmentation of ions, fragmentation reactions, Mass analyzers (Quadrople, Ion trap, ToF, Orbitrap, magnetic and electromagnetic analyzers), Ion cyclotron resonance and FT-MS.

Application of above techniques to organic chemistry and structural elucidation with exhaustive examples from latest publications.

Suggested Readings **:**

- Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan: *Introduction to Spectroscopy*, 4th Edition, Brookes Cole, **2008**.
- Harald Gunther: *NMR spectroscopy, Basic principles, concepts, and applications in chemistry*, 2nd Ed., Wiley, **2001** (reprint)
- Timothy Claridge: *High Resolution NMR Techniques in Organic Chemistry*, 2nd Ed. Elsevier, **2009**
- Edmond de Hoffmann, Vincent Stroobant: *Mass Spectrometry, Principles and applications*, 3rd Edition, Wiley, **2007**
- Robert M. Silverstein, Francis X. Webster, David Kiemle: *Spectrometric identification of organic compounds*, 7th Edition, Wiley, **2005**.

CHM 421: Statistical Mechanics (4)

Prerequisites: *CHM 222/PHY 309, CHM 322/PHY 303*

***Learning Objectives*:**

Statistical mechanics is a theoretical framework that allows establishing a bridge between the microscopic world and the behavior of macroscopic material which is amenable to experiment. The main objective of this course is to develop an understanding of the statistical nature of the laws of thermodynamics and calculate the physical properties of systems starting from the interactions between the constituent particles. We will discuss the basic principles of statistical mechanics and its applications to various physical and chemical processes in many-body systems.

***Course Contents*:**

Review of classical thermodynamics: Laws of thermodynamics and thermodynamic potentials, Legendre transforms and derivative relations, conditions of thermodynamic equilibrium and stability.

Elementary probability theory: Definition of probability, distribution functions and moments, average, variance and binomial distribution for large numbers and central limit theorem, statistical concept of uncertainty.

Fundamental principles of statistical mechanics: Macroscopic and microscopic states, fundamental postulates of statistical mechanics, statistical mechanical ensembles and their distribution functions, partition functions, entropy and Boltzmann distribution law, relation between partition functions and thermodynamic quantities in different ensembles, and fluctuations.

Ideal systems: Monatomic, diatomic and polyatomic gases and calculation of partition functions, heat capacities of gases, equipartition theorem and the Maxwell velocity distribution, Gibbs paradox, ortho- and para-hydrogen, blackbody radiation, heat capacities of solids (Einstein and Debye models), chemical equilibrium in ideal gas mixtures, photon and phonon gas systems of quantum particles and concept of different populations (Bose-Einstein and Fermi-Dirac statistics), distribution function of ideal Bose and Fermi gases, classical limits of quantum systems.

***Suggested Readings* :**

- Callen, H. B., *Thermodynamics and an Introduction to Thermostatistics*, Ed. 2nd, Wiley, **1985**.
- Hill, T. L., *An Introduction to Statistical Thermodynamics*, Dover, **1987**.
- McQuarrie, D. A., *Statistical Mechanics*, University Science Books, **2000**.
- Widom, B., *Statistical Mechanics: A Concise Introduction for Chemists,* Cambridge University Press, **2002**.
- Chandler, D., *Introduction to Modern Statistical Mechanics*, Oxford University Press, **1987.**
- Pathria, R. K., *Statistical Mechanics*, Ed. 2nd, Butterworth-Heinemann, **1996.**

CHM 422: Molecular Spectroscopy (4)

Prerequisites: *CHM 322 or PHY 303, CHM 421 or PHY 306, or their equivalent*

Basic Concepts: Nature of the electromagnetic spectrum, Born-Oppenheimer approximation, width, shape and intensity of spectral lines, Lambert-Beer law, energy levels of rigid and harmonic oscillator.

Interaction of radiation with matter: Time-dependent perturbation theory – transition amplitudes, dipoles and rates, Fermi-Golden rule, selection rules for vibrational, rotational and electronic transitions and connection to symmetry.
Microwave Spectroscopy: Moments of inertia of molecules, diatomic molecule as a rigid rotor, rotational spectra of diatomic molecules and calculation of molecular parameters, diatomic molecule as the non-rigid rotor, qualitative treatment of rotational spectra of polyatomic molecules.

Infrared Spectroscopy: Mechanism of IR absorption, vibrational spectra of diatomic molecules, diatomic molecule as an anharmonic oscillator, rotation-vibration spectra of diatomic molecules and calculation of molecular parameters, various vibrational modes in polyatomic molecules, Fermi resonance, frequency shifts because of substitutions, isotope effect, applications of IR spectroscopy in structure elucidation.

Raman Spectroscopy: Classical and quantum approach of Raman scattering, characteristic parameters of Raman lines, selection rules for Raman scattering, Raman spectra of diatomic molecules and calculation of molecular parameters, vibrational Raman spectra of polyatomic molecules and some applications.

Electronic Spectroscopy: Electronic spectra of diatomic molecules, vibrational coarse-structure, selection rules, vibrational progression, Frank-Condon principle and its consequences, theory of absorption and emission, Einstein's coefficients and their relation with transition moment integral, concept of lifetime and Einstein's spontaneous emission coefficients, symmetry properties and selection rules.

Nuclear Magnetic Resonance Spectroscopy: Nuclear spin and magnetic moment, classical and quantum mechanical description of the origin of NMR, concept of chemical shifts, effect of electron density, magnetic anisotropy, ring currents, isotope effect, lanthanide shift reagents, spin-spin coupling, coupling between groups of equivalent nuclei.

***Suggested Readings* :**

- Banwell, N., McCash, E. M., *Fundamentals of Molecular Spectroscopy*, Tata-McGraw Hill, **2007**.
- Atkins, P. W., de Paula, J., *Physical Chemistry*, Ed. 9th, Oxford Press, **2009.**
- Engel, T., *Quantum Chemistry and Spectroscopy*, Pearson Education, **2007**.
- Becker, E. D., *High Resolution NMR: Theory and Applications*, Academic Press**, 1991**.
- Wilson, E. B., Decius, J. C., and Cross, P. C., *Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra*, Dover, **1980**.
- Harris, D. C., and Bertolucci, M. D., *Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy*, Dover, **1989**.
- Steinfeld, J. I., *Molecules and Radiation: An Introduction to Modern Molecular Spectroscopy*, Ed. 2nd, Dover, **2005**.
- Berry, R. S., Rice, S. A., Ross, J., *Physical Chemistry*, Ed. 2nd, Oxford Press, **2000**.

CHM 423:Physical Chemistry Laboratory II (3)

Prerequisites: *CHM 103, CHM 222, CHM 224, CHM 321 and preferably CHM 324*

***Learning Objectives*:**

The course will aim at introducing basic as well as advanced level experiments in Physical Chemistry involving adsorption, spectrophotometry, fluorimetry, viscometry, conductometry, etc.

Suggested Experiments:

- To Verify the Freundlich and the Langmuir Adsorption Isotherms
- Determination of Fluorescence Quantum Yield of an Unknown Compound Using a Standard Fluorophore
- Determination of Critical Micelle Concentration of Sodium Dodecyl Sulphate by Fluorimetry and Correlation by Conductometry
- Determination of Average Molecular Weight of Polystyrene from Viscosity Measurements
- To determine the formula and stability constant of a complex by spectrophotometery
- Determination of the solubility curve for a ternary system of two non-miscible liquids and a third liquid which is miscible with each of them
- Determination of the solubility of benzoic acid between 25^{o}C and 60^{o}C and calculate the heat of solution
- Calibration of a given burette
- Determination of the variation of miscibility of phenol in water with temperature and estimating the Critical Solution Temperature
- To Study the Nature of the Cyclic Voltammogram for a One Electron Transfer $[Fe^{III}(CN)_6]^{3-}/[Fe^{II}(CN)_6]^{4-}$ System and Calculation of the Diffusion Coefficient of the Ion for the Given System

CHM 601: Non-transition Metal Chemistry (4)

Prerequisites: *CHM 102, CHM 301*

Concepts and principles of nontransition metal chemistry: An overview of bonding models in inorganic chemistry, Chemical forces, Bent's rule, Application of molecular orbital theory to polyatomic molecules (localized and delocalized orbitals), Walsh diagrams, Fluxional molecules, Atomic inversion, Berry pseudorotation.

The role of *p*- and *d*- orbital participation in nonmetals, Periodicity, periodic anomalies of the nonmetals, multiple bonding in heavier main group elements, charge transfer complexes.

Representative chemistry of s- and p-blocks: alkali metals, boranes, carboranes, boron clusters, Wade's rules, metallacarboranes, boron nitride nanotubes, fullerene, grapheme, CNT, organosilicon compounds, silicates and aluminosilicates, zeolites, silylenes and R_3Si+, Polysilanes, stability and activation of dinitrogen, phosphorus oxides, oxyacids, phosphines, anion chemistry of N, P, As and Sb, singlet and triplet oxygen, oxygen activation, chemistry of chalcogens, polychalcogenides, sulfur-nitrogen compounds, halogens, pseudohalogens, interhalogens, noble gases, CFC

Chemistry of carbenes, push-pull carbenes, stable heavier carbene analogues (Silicon, Germanium, Tin and lead): synthesis, characterisation and reactivity.

Multiple bonding in heavier main-group elements: Synthesis, structure and reactivity.

Main group organometallic chemistry: Preparation, stability aspects and reactions. Structurally diverse *π*-cyclopentadienyl complexes of the main group elements. Element-Element Addition to Alkynes (Si-Si, Ge-Ge, B-B, S-S, Se-Se, Ge-Sn, Si-B, Sn-B, S-B, Se-P, Si-S).

Interlocked macromolecules: catenanes, rotaxanes, pseudorotaxanes.

Suggested Readings **:**

- *Inorganic Chemistry-Principles of Structure and Reactivity.* J. E. Huheey, E. A. Keiter, R. L. Keiter, *4th Edn.* Harper-Collins, NY, **1993**.
- *Chemistry of the Elements.* N. N. Greenwood, and Earnshaw, A. *1st Edn.* Pergamon, Oxford, **1989**.
- *Concepts and Models of Inorganic Chemistry.* B. Douglas, D. McDaniel, J. Alexander, *3rd Edn.* John Wiley, New York. **1993**.
- *Advanced Inorganic Chemistry.* F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, *3rd Edn.* John Wiley and Sons Press, **1995**.
- *Modern Inorganic Chemistry.* W. L. Jolly, *2nd Edn.* McGraw-Hill, NY, **1991**.
- *Inorganic Chemistry.* D. F. Shriver, and P. W. Atkins. *3rd Edn.* Oxford University, Oxford, **1999**.
- Journal articles.

CHM 602: Applications of Modern Physical Methods (4)

Prerequisites (Desirable): *CHM 301, CHM 302*

***Learning Objectives*:**

Characterization techniques are central to synthesis of inorganic molecules. This course discusses applications of multinuclear NMR, ESR, CV, and XPES which are universal tools to investigate the structure of new molecules. In addition the course also sheds light on thermal methods namely DSC and TGA which are widely used to characterize the thermodynamic properties of solids.

***Course Contents*:**

Nuclear Magnetic Resonance Spectroscopy: Introduction, multinuclear NMR of various inorganic and organometallic compounds. [15]

Electron Paramagnetic Resonance Spectroscopy: Theory, Analysis of EPR spectra of systems in liquid phase, radicals containing single and multiple set of protons, triplet ground states. Transition metal ions, rare earth ions, ions in solid state. Double resonance techniques: ENDOR in liquid solution, powders and in non-oriented solids. [10]

Mossbauer Spectroscopy: Physical concepts, spectral line shape, isomer shift, quadrupole splitting, magnetic hyperfine interaction. Interpretation of Mossbauer parameters of ^{57}Fe and ^{119}Sn. Applications to Solid-state reactions, thermal decomposition, ligand exchange, electron transfer and isomerism. [5]

Electrochemical Methods: Heterogeneous electron transfer and concept of capacitative and Faradic current. CV, DPV and coulometry. Applications of CV in organic and inorganic chemistry. [4]

Mass Spectroscopy: Introduction and Applications to Isotopic systems. [1]

X Ray Photoelectron spectroscopy: Principles, Core level PES, Valence-electron PES, and Valence excitation spectroscopy. [4]

Thermal methods of characterization: DSC and TGA. [2]

***Suggested Readings* :**

- *NMR Spectroscopy – An Introduction*, H. Gunther, John Wiley, **1980**.
- *Inorganic Spectroscopic Methods, Alan K. Brisdon, OUP,* **2005**.
- *NMR Spectroscopy in Inorganic Chemistry,* Jonathan A.Iggo, *OUP*, **2011**.
- *NMR, NQR, EPR and Mossbauer spectroscopy in Inorganic Chemistry, R.V.Parrish, Ellis Horwood Limited, UK,* **1990**.
- *R.S.Drago Physical Methods in Inorganic Chemistry,* East-West Press Pvt. Ltd.-New Delhi,2012.
- *Structural Methods in Inorganic Chemistry*, E. A. V. Ebsworth, D. W. H. Rankin & S. Cradock, 2nd Ed.**1991**, CRC Press, Boca Raton, Florida.
- *Electrochemical methods – Fundamentals and applications*, A. J. Baird and L. R. Faulkner, Wiley, **1980**.
- *Applications of Physical Methods to Inorganic and Bioinorganic Chemistry*, R. A. Scott, C. M. Lukehart, Wiley, **2007**.

CHM 603: Advanced Inorganic Chemistry (4)

Prerequisites: *CHM 102, CHM 302*

Basics:
Quantitative discussion on bonding (MO theory, Ligand Field Theory), electronic spectra and magnetism of transition metal coordination complexes.
Thermodynamics and non-redox kinetic factors in coordination complexes.
Metal-Metal bond

New trends in transition metal coordination chemistry:
Photochemistry and photophysics of transition metal complexes.
Water splitting reaction using coordination compounds.
Crystal Engineering: Metalo-supramolecular chemistry, Metal Organic Frameworks and their applications.
Inorganic complexes as MRI contrast agents.

Suggested Readings **:**

- *Bioinorganic Photochemistry*, Stochel, G.; Brindell, M.; Macyk, W.; Stasicka, Z.; Szacilowski, K. Wiley, West Sussex, UK, **2009**.
- *Bioinorganic Chemistry*, Lippard, S. J.; Berg, J. M. University Science Books, California, **1994**.
- Discussion on above mentioned topics with relevance to the recent literature.

CHM 605: Bioinorganic Chemistry (4)

Prerequisites: *CHM 102, CHM 302*

***Learning Objectives*:**

This course highlights the significance, specific role, and working models of transition metal complexes in various important and essential biological processes.

***Course Contents*:**

Mineral Origin of life. Archaeal, Eucarial and Bacterial domain.

Transition metal ions in biology. Metallobiomolecules. Electron carriers, oxygen carriers, enzymes. environment.

Specific examples: Hemoglobin, Myoglobin, Hemocyanin, Hemrythrin cytochromes, Fe-S proteins, Cytochrome P-450, Nitrophorin, NO-synthase, peroxidase, catalase, Ferritin, cytochrome-C oxidase, cerulplasmin, blue copper proteins, *di*- and *tri*-copper proteins. Other enzymes like, hydrogenase, methane monooxygenase, dioxygenases, dehydratase, nitrogenase, molybdenum containing oxidase and reductase class of enzymes like sulfite oxidase, xanthine oxidase, nitrate reductase, DMSO reductase, tungsten containing formate dehydrogenase and tungsten bearing hyperthermophilic and thermophilic enzymes. Zn enzymes like carbonic anhydrase, carboxypeptidase, DNA and RNA polymerases, Nickel containing F-430, role of manganese in water splitting.

Active site analogue reaction models and structural models of these enzymes.

Environmental chemistry, auto exhaust, arsenic and other heavy metal pollutions.

Forensic chemistry; inorganic chemistry in medicine, platinum complexes, Mo=S complexes as anti-cancer drugs.

Biochemistry of main group elements.

***Suggested Readings* :**

- *Principles of Bioinorganic Chemistry*, S. J. Lippard, J. M. Berg, University Science Books, **1994**.
- *Bioinorganic Chemistry*, I. Bertini, H. B. Gray, S. J. Lippard, S. J. Valentine, Viva Books, 1st Edition, **1998**.

CHM 607: X-ray diffraction: Principles and Applications (4)

***Learning Objectives*:**

The understanding of the three dimensional arrangement of atoms in crystalline solids and their relationship to chemical and biological function.

***Course Contents*:**

Prerequisites: *CHM 301; may be removed for other students subject to Instructor's discretion*

Symmetry in the Solid State: Unit Cell, Crystal Systems, Crystal lattices (2D), Bravais Lattices (3D), Miller planes (crystallographic directions and multiplicities), d-spacing formula (resolution), Point Symmetry and Point Groups, Space groups (equivalent points, Wyckoff positions, site occupancy factor).

Elements of X-ray diffraction: Thomson and Compton Scattering, Interference of Scattered Waves, Scattering by an Atom and Crystal, Bragg's Law, Reciprocal Lattice, Reflecting and Limiting sphere of reflection.

Preliminary concepts on Crystals and X-rays

Intensity and Geometric Data Collection and Reduction statistics, Factors that affect intensities (Lorentz and Polarization corrections), Interpretation of Intensity data, Wilson plot and absolute scale factor.

Theory of Structure Factors and Fourier Synthesis: Calculation of Structure Factor amplitudes (general formula and applications), Friedel's Law, Systematically absent reflections, Anomalous Dispersion

Structure Solution and refinement: Patterson symmetry, Direct Methods, Least Squares Methods, Electron density maps, R-factors, refinement by DF synthesis.

Crystal structure determination: Asymmetric Unit, crystal density, unit cell contents, and chemical formula. Thermal Motion, the physical interpretation of molecular (Bond lengths, angles and torsions) and crystal structure (Packing Diagram), Rietveld method in Powder diffraction.

Suggested Readings **:**

- *A Basic Course in Crystallography:* J. A. K. Tareen & T. R. N. Kutty.
- *Fundamentals of Crystallography:* C. Giacavazzo.
- *Basics of Crystallography and Diffraction:* C. Hammond.
- *X-ray Structure determination:* A practical guide: G. H. Stout and L. H. Jensen.

CHM 609: Transition Metal Organometallic Chemistry (4)

Prerequisites: *CHM 102, CHM 301, CHM 302*

Structure and bonding: Brief overview of transition metal orbitals, electron counting, formal oxidation state, 18-e rule and its exceptions, isoelectronic and isolobal analogies, common geometries for transition metal complexes (Crystal Field Theory, MO description), σ- and π-bonding, types of ligands and their properties, soft vs hard ligands.

Reactions of organometallic complexes: ligand substitution/ exchange/dissociation processes and thermochemical considerations, catalyzed and assisted ligand substitution reactions, oxidative addition (definition, mechanism, thermodynamic consideration), oxidative addition of non-polar and polar electrophilic reagents, reductive elimination (bite angle effects, π-acid effects), transmetallation (definition, mechanism, utility), insertion/de-insertion, nucleophilic and electrophilic attack on coordinated ligands.

Complexes with classic Lewis base donors: Amines, phosphines and other related donors.

Complexes with metal-carbon σ-bonds: **(a)** Metal carbonyl complexes: Synthesis, structure and bonding; IR spectroscopy; Reactions; Related complexes with cyanide, nitrosyl, and dinitrogen ligands. **(b)** Metal alkyl complexes: Synthesis, stability and structure; Reactions; Activation of C-H bonds. **(c)** Alkylidene and alkylidyne complexes: Synthesis; structure and bonding; Reactivity; Olefin metathesis.

Metal-element multiple-bonded complexes: Oxo, sulfido, imido, hydroazido, nitrido-complexes: Synthesis, bonding, structure, spectroscopy, and reactivity.

Complexes with metal-metal multiple bonds: Synthesis, structure and bonding, spectroscopic and magnetic properties, and reactions.

Metal complexes of π-ligands: **(a)** Alkene complexes: Synthesis; Bonding; Reactivity. **(b)** Alkyne complexes: Synthesis; Bonding; Reactivity. **(c)** Cyclopentadienyl complexes: Discovery of 'sandwich' complexes; Bonding; Properties of Cp complexes of 3d metals; Substituted metallocenes; Zigler-Natta polymerization; Half-sandwich complexes. **(d)** Allyl and dienyl complexes: Synthesis; Structure and properties; Reactivity. **(e)** Arene complexes: Bis-arene complexes; Arene half-sandwich complexes; η^2 to η^4 coordinated arenes; Seven and eight-membered ring ligands.

Modern applications of organometallic chemistry: **(a)** Small molecule activation and functionalization: mechanistic and practical view. **(b)** Organometallic materials.

***Suggested Readings* :**

- Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals,* 3rd Ed.; Wiley-Interscience: New York, **2001**.
- Hartwig, J. F. *Organotransition Metal Chemistry From Bonding to Catalysis,* 1st Ed.; University Science Books: Sausalito, CA, **2010**.
- Collman, J.P.; Hegedus, L.S.; Norton, J.R.; Finke, R.G. *Principles and Applications of Organotransition Metal Chemistry*; University Science: Mill Valley, CA, **1987**.
- Spessard, G.O.; Miessler, G.L. *Organometallic Chemistry*. Prentice Hall: Upper Saddle River, NJ, **1996**.
- Huheey, J.E.; Keiter, E.A.; Keiter, R.L. *Inorganic Chemistry: Principles of Structure and Reactivity,* 4th Ed.; HarperCollins: New York, **1993**.

- Jordan, R. B. *Reaction Mechanisms of Inorganic and Organometallic Systems;*2nd Ed.; Oxford University Press: Oxford, **1998**.
- (a) Bochmann, M. *Organometallics 1;* Oxford University Press: New York, 1994. (b) Bochmann, M. *Organometallics 2;* Oxford University Press: New York, **1994**.
- Elschenbroich, C.; Salzer, A. *Organometallics: A Concise Introduction,* 2nd Ed.; VCH: New York, **1992**.
- Shriver, D. F.; Atkins, P. W. *Inorganic Chemistry,* 3rd Ed.; W. H. Freeman: New York, **1999**.
- Attwood, J. D. *Inorganic and Organometallic Reaction Mechanisms,* 2nd Ed.; VCH Publishers Inc.: New York, **1997**.
- Nugent, W. A.; Mayer, J. A. *Metal-Ligand Multiple Bonds,* 1st Ed.; Wiley-Interscience, **1987**.
- Elschenbroich, C. *Organometallics, 3rd, Completely Revised and Extended Edition;*Wiley-VCH Verlag GbmH & Co. KGaA, Weinheim, Germany, **2006**.
- Cotton, F. A.; Murillo, C. A.; Walton, R. A. *Multiple Bonds between Metal Atoms,* 3rd Ed.; Springer Science Inc. New York, **2005**.
- Primary literature (journal articles).

CHM 611: Physical Organic Chemistry (4)

Prerequisites: *CHM 311, CHM 312*

Chemical Equilibria and Chemical Reactivity:

- Thermodynamic and kinetic control of reactions
- Correlation of reactivity with structure, linear free energy relationships, Hammond's postulate, Curtin-Hammett principle, substituent constants and reaction constants

Chemical Kinetics and Isotope Effects:

- Various types of catalysis and isotope effects, importance in the elucidation of organic reaction mechanisms

Stereoelectronic Effects in Organic Chemistry:

- Role of stereoelectronic effects in the reactivity of acetals, esters, amides and related functional groups
- Reactions at sp^3, sp^2, and sp carbons, Cram, Felkin-Ahn, Zimmerman-Traxler, Houk, Cieplak, exterior frontier orbital extension (EFOE) and cation-complexation models as applied to p-facial stereoselectivity
- Allylic strain ($A^{1,2}$ and $A^{1,3}$) and other strains

Pericyclic Reactions:

- Conservation of orbital symmetry, Woodward-Hoffmann rules, frontier molecular orbital (FMO) theory
- Orbital overlap effects in cycloadditions, electrocyclizations, sigmatropic rearrangements and chelotropic reactions
- Paterno-Buchi, Norrish type I and II reactions

Suggested Readings **:**

- Isaacs, N. S. *Physical Organic Chemistry*, Prentice Hall, **1996**.
- Deslongchamps, P. *Stereolectronic Effects in Organic Chemistry*, Elsevier Science, **1983**.
- Carey, F. A., Sundberg, R. J. *Advanced Organic Chemistry*, *Part A and B*, Springer, **2007**.
- Turro, N. J. *Modern Molecular Photochemistry*, University Science Books, **1991**.
- Anslyn, E. V., Dougherty, D. A. *Modern Physical Organic Chemistry*, University Science Books, **2005**.
- Woodward, R. B., Hoffmann, R. *The Conservation of Orbital Symmetry*, Verlag Chemie, **1970**.
- Lehr, R. E., Marchand, A. P. *Orbital Symmetry: A Problem Solving Approach*, Academic Press, **1972**.

CHM 612: Advanced Organic Chemistry II (4)

Prerequisites: *CHM 311, CHM 312*

Reactions related to synthesis of 3 to 6 membered and higher carbocycles.

Miscellaneous reactions: (a) tandem/domino reaction, (b) multicomponent reaction (MCR), (c) remote functionalization.

Philosophy of synthetic design: Retrosynthesis, importance of reactivity, relation between functional groups, regio and stereocontrol, use of functional groups as a guide for retrosynthesis.

Concepts of atom, step and redox economy.

Total synthesis of natural products.

Suggested Readings **:**

- Clayden, J., Greeves, N., Warren, S., Wothers, S. *Organic Chemistry*, Oxford University Press, **2001**.
- Wyatt, P., Warren, S. *Organic Synthesis: Strategy and Control*, Wiley, **2007**.
- Warren, S. *Organic Synthesis: The Disconnection Approach*, Wiley, **1983**.
- Nicolaou, K. C., Sorensen, E. *Classics in Total Synthesis*, Wiley-VCH, **2008**.
- Nicolaou, K. C., Snyder, S. A. *Classics in Total Synthesis-II*, Wiley-VCH, **2003**.
- Corey, E. J., Cheng, X-M. *The Logic of Chemical Synthesis*, Wiley, **1995**.

CHM 613: Advanced Organic Chemistry I (4)

Prerequisites: *CHM 311, CHM 312*

***Learning Objectives*:**

This is an advanced level course where students would learn asymmetric construction of C-C and C-hetero bond-forming reactions. Various aspects of asymmetric synthesis such as basic principle of enantioselective reactions, dynamic kinetic asymmetric transformations (DYKAT), synthesis of enantioenriched organic compounds via resolutions (kinetic, parallel kinetic, and dynamic kinetic resolutions), and various diastereoselective processes would be taught is this course.

***Course Contents*:**

Concepts and principles of enantioselective and diastereoselective transformations (including Curtin-Hammet principle, 1,2-induction and 1,3-induction models)

Asymmetric C-C bond forming reactions (Asymmetric alkylations, Asymmetric additions to C=O, C=N, C=C bonds)

Asymmetric oxidation reactions (Dihydroxylations, epoxidations, enolate oxidations, chiral sulfoxides, etc.)

Asymmetric reductions of C=C, C=O and C=N bonds.

Resolutions (Kinetic, Parallel Kinetic, Dynamic Kinetic resolutions)

Non-linear effects and autocatalysis.

Desymmetrization reactions

Introduction to Organocatalysis (Covalent and non-covalent catalysis)

***Suggested Readings* :**

- Walsh, P. J., Kozlowski, M. C. *Fundamentals of Asymmetric Catalysis*, University Science Book, **2009**.
- Ojima, I. *Catalysis in Asymmetric Synthesis*, Wiley-VCH, **2004**.
- Carreira, E., Kvaermo, L. *Classics in Stereoselective Synthesis*, Wiley-VCH, **2009**.
- Berkessel, A., Groger, H. *Asymmetric Organocatalysis: From Biomimetic Concepts to Applications in Asymmetric Synthesis,* Wiley-VCH, **2005**.
- Hassner, A. *Advances in* ***Asymmetric Synthesis,*** Vol 3, Elsevier, **1999**.

CHM 614: Advanced Organic Chemistry III (4)

Prerequisites: *CHM 311, CHM 312*

Concepts (Ligand systems, electron counting and chemical bonding).

Fundamental aspects (ligand substitutions, oxidative addition/reductive elimination, intramolecular insertions/ eliminations, nucleophilic/ electrophilic addition on coordinated ligands).

Coupling reactions and their synthetic applications (C-C and C-Heteroatom bond forming reactions).

Brief introduction to Fischer and Schrock carbene complexes, Metathesis (concepts and catalysts, RCM, ROM, CM, yne-metathesis, ene-yne metathesis and their applications).

Miscellaneous transition metal catalyzed reactions (C-H and C-F bond activation, carbonylation, click chemistry, hydrosilylation, etc.)

Suggested Readings **:**

- Crabtree, R. H. *The organometallic chemistry of the transition metals*, John Wiley, **2005**.
- Hegedus, L. S. *Transition metals in the synthesis of complex organic molecule*, University Science Books, **2010** (3rd Ed).
- Grubbs, R. H. (Editor) *Handbook of Metathesis*, (Vol 1-3), Wiley-VCH, **2003**.
- Hartwig, J. H. *Organotransition Metal Chemistry: From Bonding to Catalysis*, University Science Books, **2009** (1st Ed).

CHM 615: Frontiers in Organic Chemistry (4)

Prerequisites: *CHM 311, CHM 312*

In this course, ***most recent advances in areas of organic chemistry*** will be discussed.

The emphasis will be to discuss ***latest research papers*** and also those published in the ***last 5 years*** so as to give an in-depth exposure to the latest advances in organic synthesis.

Suggested Readings **:**

- Research article published in National and International journals.
- Carriera, E. M.; Kvaerno, L. *Classics in Stereoselective synthesis*, Wiley-VCH.
- Hudlicky, T.; Reed, J. W. *The Way of Synthesis*, Wiley-VCH.
- Kurti, L.; Czako, B. *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier.
- Nicolaou, K. C., Sorensen, E. *Classics in Total Synthesis*, Wiley-VCH.
- Nicolaou, K. C., Snyder, S. A. *Classics in Total Synthesis-II*, Wiley-VCH.

CHM 616: Spectroscopy and its Application to Organic Molecules (4)

Prerequisites: *CHM 311, CHM 312*

Infrared spectroscopy: Theory of IR spectroscopy, Modes of stretching and bending, Fourier Transform Spectrometers, Background spectrum, Survey of important functional groups with examples, Chemical environment and chemical shift.

Nuclear Magnetic Resonance: Physical basis of Nuclear Magnetic Resonance spectroscopy, Chemical shift and Spin-spin coupling as functions of structure, Analysis of high-resolution NMR spectra, FT and pulse-NMR, NOE, 2D NMR (COSY, INADEQUATE, HMQC, HSQC, HMBC, NOESY, HETCOR, ROESY, TOCSY).

Mass spectroscopy: Principles of Mass Spectrometry, Ion sources (EI, CI, Field Ionization, FAB, Plasma desorption, Field desorption, Laser desorption, MALDI, Thermospray, API, ESI, APCI, APPI, Atmospheric pressure secondary ion mass spectrometry, inorganic ionization techniques, formation and fragmentation of ions, fragmentation reactions, Mass analyzers (Quadrople, Ion trap, ToF, Orbitrap, magnetic and electromagnetic analyzers), Ion cyclotron resonance and FT-MS.

Application of above techniques to organic chemistry and structural elucidation with exhaustive examples from latest publications.

Suggested Readings **:**

- Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan: *Introduction to Spectroscopy*, 4th Edition, Brookes Cole, **2008**.
- Harald Gunther: *NMR spectroscopy, Basic principles, concepts, and applications in chemistry*, 2nd Ed., Wiley, **2001** (reprint)
- Timothy Claridge: *High Resolution NMR Techniques in Organic Chemistry*, 2nd Ed. Elsevier, **2009**
- Edmond de Hoffmann, Vincent Stroobant: *Mass Spectrometry, Principles and applications*, 3rd Edition, Wiley, **2007**
- Robert M. Silverstein, Francis X. Webster, David Kiemle: *Spectrometric identification of organic compounds*, 7th Edition, Wiley, **2005**.

CHM 617: Chemical Biology (4)

Prerequisites: *CHM 343*

Introduction: What is Chemical Biology, Basics of Biology: Lipids, DNA, Protein, Sugars - their function and importance.

Structure of peptides and proteins: Primary, secondary and tertiary structure, Non-covalent interactions, Aggregation, Folding, Misfolding.

Microscopy and Spectroscopy in Biology: AFM, SEM, TEM, DLS, CD, UV-Vis, Fluorescence and Bioluminescence, NMR, MS.

Bioorthogonal Ligation techniques: Functional group specific ligation techniques, Strategies for attachment of synthetic molecules to biomolecules, Bioorthogonal ligations, Staudinger Ligation, Native Chemical Ligation, Intein-mediated synthesis, Site selective protein modification.

Natural and Synthetic Lipids**:** Natural and synthetic membranes, Vesicles. Designing synthetic vectors for DNA and siRNA, Differential Scanning Calorimetry.

DNA chemistry and its uses:Molecular recognition of DNA**,** Recognition and modulation of DNA, RNA, and proteins with small molecules, siRNA, RNAi and its applications, DNA-based architectures and DNA Nanotechnology.

Suggested Readings **:**

- Herbert Waldmann, *Chemical Biology: Learning Through Case Studies*; Wiley-VCH, Weinheim **2009**.
- Dobson, Gerrard & Pratt, *Foundations of Chemical Biology*; Oxford Univ. Press; **2002**.
- Miller & Tanner, *Essentials Of Chemical Biology: Structure and Dynamics of Biological Macromolecules*; Wiley; **2002**.
- Waldman & Janning, *Chemical Biology: A Practical Course*; Wiley-VCH; **2004**.
- Greg T. Hermanson, *Bioconjugate Techniques*; Academic Press, **2008**.
- Joseph R. Lackowicz, *Principles of Fluorescence Spectroscopy*; Springer; **2006**.
- Journal Articles

CHM 621: Statistical Mechanics (4)

Prerequisites: *CHM 222/PHY 309, CHM 322/PHY 303*

Review of classical thermodynamics: Laws of thermodynamics and thermodynamic potentials, Legendre transforms and derivative relations, conditions of thermodynamic equilibrium and stability.

Elementary probability theory: Definition of probability, distribution functions and moments, average, variance and binomial distribution for large numbers and central limit theorem, statistical concept of uncertainty.

Fundamental principles of statistical mechanics: Macroscopic and microscopic states, fundamental postulates of statistical mechanics, statistical mechanical ensembles and their distribution functions, partition functions, entropy and Boltzmann distribution law, relation between partition functions and thermodynamic quantities in different ensembles, and fluctuations.

Ideal systems: Monatomic, diatomic and polyatomic gases and calculation of partition functions, heat capacities of gases, equipartition theorem and the Maxwell velocity distribution, Gibbs paradox, ortho- and para-hydrogen, blackbody radiation, heat capacities of solids (Einstein and Debye models), chemical equilibrium in ideal gas mixtures, photon and phonon gas systems of quantum particles and concept of different populations (Bose-Einstein and Fermi-Dirac statistics), distribution function of ideal Bose and Fermi gases, classical limits of quantum systems.

Suggested Readings **:**

- Callen, H. B., *Thermodynamics and an Introduction to Thermostatistics*, Ed. 2nd, Wiley, **1985**.
- Hill, T. L., *An Introduction to Statistical Thermodynamics*, Dover, **1987**.
- McQuarrie, D. A., *Statistical Mechanics*, University Science Books, **2000**.
- Widom, B., *Statistical Mechanics: A Concise Introduction for Chemists,* Cambridge University Press, **2002**.
- Chandler, D., *Introduction to Modern Statistical Mechanics*, Oxford University Press, **1987.**
- Pathria, R. K., *Statistical Mechanics*, Ed. 2nd, Butterworth-Heinemann, **1996.**

CHM 622: Molecular Spectroscopy (4)

Prerequisites: *CHM 322 or PHY 303, CHM 421 or PHY 306, or their equivalent*

Basic Concepts: Nature of the electromagnetic spectrum, Born-Oppenheimer approximation, width, shape and intensity of spectral lines, Lambert-Beer law, energy levels of rigid and harmonic oscillator.

Interaction of radiation with matter: Time-dependent perturbation theory – transition amplitudes, dipoles and rates, Fermi-Golden rule, selection rules for vibrational, rotational and electronic transitions and connection to symmetry. *Microwave Spectroscopy:* Moments of inertia of molecules, diatomic molecule as a rigid rotor, rotational spectra of diatomic molecules and calculation of molecular parameters, diatomic molecule as the non-rigid rotor, qualitative treatment of rotational spectra of polyatomic molecules.

Infrared Spectroscopy: Mechanism of IR absorption, vibrational spectra of diatomic molecules, diatomic molecule as an anharmonic oscillator, rotation-vibration spectra of diatomic molecules and calculation of molecular parameters, various vibrational modes in polyatomic molecules, Fermi resonance, frequency shifts because of substitutions, isotope effect, applications of IR spectroscopy in structure elucidation.

Raman Spectroscopy: Classical and quantum approach of Raman scattering, characteristic parameters of Raman lines, selection rules for Raman scattering, Raman spectra of diatomic molecules and calculation of molecular parameters, vibrational Raman spectra of polyatomic molecules and some applications.

Electronic Spectroscopy: Electronic spectra of diatomic molecules, vibrational coarse-structure, selection rules, vibrational progression, Frank-Condon principle and its consequences, theory of absorption and emission, Einstein's coefficients and their relation with transition moment integral, concept of lifetime and Einstein's spontaneous emission coefficients, symmetry properties and selection rules.

Nuclear Magnetic Resonance Spectroscopy: Nuclear spin and magnetic moment, classical and quantum mechanical description of the origin of NMR, concept of chemical shifts, effect of electron density, magnetic anisotropy, ring currents, isotope effect, lanthanide shift reagents, spin-spin coupling, coupling between groups of equivalent nuclei.

***Suggested Readings* :**

- Banwell, N., McCash, E. M., *Fundamentals of Molecular Spectroscopy*, Tata-McGraw Hill, **2007**.
- Atkins, P. W., de Paula, J., *Physical Chemistry*, Ed. 9th, Oxford Press, **2009.**
- Engel, T., *Quantum Chemistry and Spectroscopy*, Pearson Education, **2007**.
- Becker, E. D., *High Resolution NMR: Theory and Applications*, Academic Press**, 1991**.
- Wilson, E. B., Decius, J. C., and Cross, P. C., *Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra*, Dover, **1980**.
- Harris, D. C., and Bertolucci, M. D., *Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy*, Dover, **1989**.
- Steinfeld, J. I., *Molecules and Radiation: An Introduction to Modern Molecular Spectroscopy*, Ed. 2nd, Dover, **2005**.
- Berry, R. S., Rice, S. A., Ross, J., *Physical Chemistry*, Ed. 2nd, Oxford Press, **2000**.

CHM 624: Molecular Simulations (4)

Prerequisites: *CHM222/PHY309, CHM322/PHY303, CHM421/PHY306 or equivalent*

Introduction to scientific programming, brief overview of molecular simulation methods and their application.

Concept of phase space, statistical ensembles and averages, fluctuations, phase space distribution functions and the Liouville equation.

Born-Oppenheimer approximation, potential energy surfaces, brief overview of Hartree-Fock theory and the density functional theory, Hellman-Feynman theorem.

Description of semi-empirical force-fields and parameterization, techniques for energy minimization and normal mode analysis.

Molecular Dynamics (MD):

- Introduction to molecular dynamics, equations of motion, approximate integration schemes, force calculations, initialization and boundary conditions, potential truncation, stability, simulation of bulk phases with continuous potentials, evaluation of thermodynamic and transport properties.
- Extended Lagrangian, thermostats and barostats, methods of constraints, multiple time-steps. Methods for treating long-range Coulomb interactions, ab-initio molecular dynamics.

Monte Carlo (MC):

- Introduction, importance sampling, Markov chains and detailed balance, Metropolis method.
- Extension to various ensembles (canonical, isothermal-isobaric, grand-canonical, and Gibbs ensemble). Monte Carlo simulation of monatomic fluids and complex molecules, study of phase-equilibria.

Further Advanced Topics and Applications:

- Methods for calculation of free energy, solvation models for use with empirical potentials, advanced sampling techniques and rare events, combined quantum mechanical/molecular mechanical (QM/MM) methods, coarse-graining and mesoscale simulation methods.
- Brief introduction to commercial simulation software.

***Suggested Readings* :**

- *Molecular Modelling – Principles and Applications*, A. R. Leach, 2nd Ed., Prentice Hall, 2001.
- *Understanding Molecular Simulation*s, D. Frenkel and B. Smit, 2ndEd., Academic Press, 2002.
- *Computer Simulation of Liquids*, M. P. Allen and D. J. Tildesley, Oxford,1987.
- *Essentials of Computational Chemistry: Theories and Models*, C. J. Cramer, 2nd Ed., Wiley, 2004.

CHM 625: Biophysical chemistry (4)

Prerequisites: *CHM222/PHY309, CHM 321, CHM322/PHY303, CHM421/CHM621/PHY306/PHY621, PHY304/604 or equivalent*

***Learning Objectives*:**

The prime objective of this course is to understand structure and dynamical properties of biomolecules, forces responsible for biological processes. Understanding structure function relationship of biomolecules using various instrumental techniques is also one of the main learning objectives of this course.

***Course Contents*:**

*Structure of Proteins and Nucleic Acids***:** Primary and secondary structure, Ramachandran plot, conformational analysis, tertiary structure, structure of a nucleotide chain, the DNA double helix model, polymorphism.

Molecular Forces in Biological Structures: Electrostatic interactions, hydrophobic and hydrophilic forces, hydrogen bonding interactions, ionic interactions, stabilizing forces in proteins and nucleic acids, steric interactions.

Configurational Statistics of Biomacromolecules: End-to-end distance and radius of gyration of a polymer chain, statistics of random coils, persistence length, rotational isomeric state model, helix-coil transition and the Zimm-Bragg model, cooperativity in ligand binding and folding, allosteric transitions.

Dynamics of Biomacromolecules: Brownian motion and the random walk model, Fick's law of diffusion, friction and diffusion coefficients, Langevin equation and time correlation functions, Kramer's theory of crossing a potential barrier.

Techniques to Study Structure-Function Inter-relationships: Applications of CD, fluorescence, NMR in characterizing biomolecular systems, use of FRET in understanding conformational dynamics.

***Suggested Readings* :**

- Cantor, C. R., and Schimmel, P., *Biophysical Chemistry (parts I, II and III)*, W. H. Freeman, **1980**.
- Jackson, M. B., *Molecular and Cellular Biophysics*, Cambridge, **2006**.
- Serdyuk, I. N., Zaccai, N. R.,and Zaccai, J.,*Methods in Molecular Biophysics: Structure, Dynamics*, *Function*, Cambridge, **2007**.
- Daune, M., *Molecular Biophysics: Structures in Motion*, Oxford, **199**9.
- Lakowicz, J. R., *Principles of Fluorescence Spectroscopy*, Plenum Press, **2003**.

CHM 626: Physical Photochemistry (4)

Prerequisites: *CHM 422/622*

Introduction to absorption: Lambert-Beer law and its deviation relation between molar extinction coefficient and absorption cross section, Einstein induced absorption coefficient and integrated Einstein induced coefficients, notation of energy levels and electronic transitions

Fluorescence: introduction, Jablonski diagram, kinetic parameters, Einstein's induced and spontaneous emission coefficients, relationship between lifetime and Einstein coefficients (Strickler and Berg' equation) and its limitations, fluorescence quantum yield, Stoke's shift, fluorescence excitation spectrum

Effects of solvents on the fluorescence spectrum: (general effects and specific effects, derivation of the equation), time scales of molecular processes in solutions, applications

Fluorescence quenching: Different mechanism of fluorescence quenching, applications

Radiationless processes: Mechanism for internal and intersystem crossing, effect of temperature of radiationless processes

Phosphorescence: kinetic parameters, origin of triplet state and its formation, different methods of triplet-triplet absorption Fluorescence Anisotropy and its applications

Resonance Energy Transfer: Different mechanisms of energy transfer (Forster and Dexter mechanism), selection rules for energy transfer, non-vertical energy transfer, Forster Resonance Energy Transfer (FRET), typical examples and choice of dyes

Spectrophotometry and Fluorometry: principles and instrumentation; choice of light sources, monochromators, choice of optical filters and various detector systems used, Concept of Time Correlated Single Photon Counting: Basic principles and instrumentation

Fluorophores and dyes used in spectroscopy: intrinsic and extrinsic fluorophores, protein labeling.

Suggested Readings **:**

- Lakowicz, J. R., Principles of Fluorescence Spectroscopy; Ed. 3rd, Plenum Press, 2003.
- Birks, J. B., "Photophysics of Aromatic Molecules"; Wiley-Interscience, 1970.
- N. J. Turro, N. J., Ramamurthy, V., J. C. Scaiano, J. C., Principles of Molecular Photochemistry: An Introduction, University Science Books, California.
- C. A. Parker; "Photoluminescence of Solutions"; Elsevier Publishing Company, 1968.

CHM 628: Electrochemistry: Fundamentals and Applications (4)

Prerequisites: *CHM 321*

Introduction and Overview of Electrode processes: Electrochemical Cells and Reactions, Nature of Electrode-Solution Interface, Faradaic Reactions, Mass Transfer Controlled Reactions, Coupled Chemical Reactions.

Electrochemical Thermodynamics: Basics of Electrochemical Thermodynamics, Liquid Junction Potentials.

Kinetics of Electrochemical Reactions: Arrhenius Equation, Transition state theory, Butler Volmer model, Marcus Theory.

Electrochemical Methods: Linear Sweep Voltammetry, Cyclic Voltammetry, Square wave Voltammetry, Chronoamperometry, Chronopotentiometry, Rotating Disk Electrode, Rotating Ring-disk Electrode, AC impedance, Spectroelectrochemistry.

Applications of Electrochemistry: Electron Transfer, Characterization of Inorganic Complexes, Catalysis, Supercapacitors and Batteries.

Suggested Readings **:**

- Electrochemical Methods: Fundamentals and Applications, Allen J Bard and Larry R. Faulkner, 2nd Edition, John Wiley and Sons
- Modern Electrochemistry Ionics: Volume 1, John O'M. Bockris and Amulya K. N. Reddy, 2nd Edition, Plenum Press.
- Recent Research Publications.

CHM 629: Advanced Molecular Spectroscopy (4)

Prerequisites: *CHM 322/642, CHM 422/622 or their equivalent*

Basic Concepts: Einstein's coefficients and their relation with transition moment integral, time-dependent perturbation theory, various kinds of transitions and selection rules, notations of energy levels and electronic transitions

Fluorescence: Introduction, Jablonskii diagram, kinetic parameters, relationship between lifetime and Einstein's coefficients (Strickler and Berg equation) and its limitations, fluorescence quantum yield, Stokes' shift, analysis of a fluorescence spectrum, effect of solvent on fluorescence, (general effects and specific effects), Lippert equation and its applications, fluorescence excitation spectra, time scales of molecular processes, fluorescence quenching, different types of mechanisms associated with fluorescence quenching and their applications, fluorescence anisotropy and its applications

Radiationless processes: Mechanism of internal conversion and inter-system crossing, effect of temperature on radiationless processes

Phosphorescence: Kinetic parameters, origin of triplet state and its formation, different methods of triplet-triplet absorption, factors affecting the rate of phosphorescence

Resonance Energy Transfer: Different mechanisms of energy transfer (Forster and Dexter), selection rules for energy transfer, non-vertical energy transfer, FRET and its applications, typical examples and choice of dyes.

Spectrophotometry and Fluorometry: Principles and instrumentation, choice of light sources and detectors, monochromators, optical filters and choice of filters, fluorophores and dyes used in spectroscopy, intrinsic and extrinsic fluorophores, protein labeling

Lasers and its applications: Principles of lasers, multi-photon ionization processes in molecules, dynamics of reactions in liquids, spectroscopy of single molecules, concept of time-resolved spectroscopy, Confocal microscopy, FCS and FLIM.

Suggested Readings **:**

- Atkins, P. W., and de, Paula, J., *Physical Chemistry*, 8th Edition, Oxford Press, **2008.**
- Levine, I., *Physical Chemistry*, McGraw-Hill, **2008**.
- Lakowicz, J. R., *Principles of Fluorescence Spectroscopy*, Plenum Press, **2003**.
- Dogra, S. K., and Randhawa, H. S.; *Atom, Moleculeand Spectrum*, New Age International Pvt. Ltd., **2011**.
- Turro, N. J., Ramamurthy, V., and Scaiano, J. C., *Principles of Molecular Photochemistry: An Introduction*, University Science Books, **2009**.
- Selvin, P. R., and Ha, T., *Single Molecule Techniques: A Laboratory Manual*, Cold Spring HarborLaboratory Press, **2008**.

CHM 630: Advanced Statistical Mechanics (4)

Prerequisites: *CHM322/CHM642/PHY303, CHM421/PHY306 or their equivalent*

Basic postulates and ensembles: Distributions, partition functions and calculation of thermodynamic properties in various ensembles.

Classical Statistical Mechanics: Classical partition function (rotational, vibrational and translational) as the high-temperature limit of its quantum counterpart, microscopic equations of motion, phase space, phase space vectors and Liouville's theorem, the Liouville equation and equilibrium solutions, ergodic theory.

Theory of imperfect gases: Cluster expansion for a classical gas, evaluation of cluster integrals, virial explansion of the equation of state, evaluation of the virial coefficients, law of corresponding states.

Theory of the liquid state: Definition of distribution and correlation functions, radial distribution function, Kirkwood integral equation, potential of mean force and the superposition approximation, Ornstein-Zernicke equation, Percus-Yevick and hypernetted-chain approximations., density expansion of the pair functions, perturbation theory of the van der Waals' equation.

Critical phenomena: Critical behaviour of the van der Waals equation, Ising model, lattice-gas model and binary alloys, broken symmetries, mean-field theories, Landau-Ginsburg theory, scaling and universality, introduction to renormalization group theory.

Suggested Readings **:**

- Chandler, D., *Introduction to Modern Statistical Mechanics*, Oxford, **1987**.
- McQuarrie, D. A., *Statistical Mechanics*, University Science Books, **2000**.
- Hansen, J. P., and McDonald, I. R., *Theory of Simple Liquids,* Ed. 3rd, Academic Press, **2006**.
- Pathria, R. K., *Statistical Mechanics*, Ed. 2nd, Butterworth-Heinemann, **1996**.
- Stanley, H. E., *Introduction to Phase Transitions and Critical Phenomena*, Oxford, **1971**.

CHM 631: Electronic Structure (4)

Prerequisites: *CHM 633*

Review of quantum chemistry – Molecular Schrodinger equation, Born-Oppenheimer approximation, variational principle, many-electron wavefunctions, Hartree-Fock theory and electron correlation.

Some early density-functional theories– Thomas-Fermi model, Slater approximation of Hartree-Fock.

Modern Density-functional theory – Introduction to functionals and functional calculus, Hohenberg-Kohn theorems, Kohn-Sham approach, meaning and utility of the Kohn-Sham orbitals and eigenvalues, approximate exchange-correlation functions.

Practical DFT – Introduction to basis sets – localized and periodic basis sets, all-electron versus pseudopotential approximations, self-consistent methods to solve the Kohn-Sham equations. Hellmann-Feynman theorem and computation of forces, computation of electronic and structural properties.

Introduction to a DFT code and some simple examples and case-studies

Suggested Readings **:**

- W. Koch and M. Holthausen, *A chemist's guide to density-functional theory*.
- A. Szabo and N. S. Ostlund., *Modern Quantum Chemistry*.
- R. Martin, *Electronic Structure.* R.G. Parr and W. Yang, *Density-functional theory of Atoms and Molecules.*

CHM 632: Physical Chemistry of Polymers (4)

Prerequisites: *CHM 222, CHM 321, CHM 324 and CHM 421 or their equivalent are desirable*

Introduction: Basic concepts, types of polymers, molecular weights, determination of molecular weights.

Polymerization kinetics: Stepwise & chain growth kinetics, Carothers equation, kinetic chain length, copolymerization and emulsion polymerization.

Structure of Polymer Chain: Chain isomerism, stereoregularity, configurations, and conformations, NMR characterizations, radius of gyration.

Polymer solutions and blends: Thermodynamics and statistical thermodynamics, lattice model, Flory-Huggins theory, osmotic pressure, phase separation, properties of dilute polymer solutions: intrinsic viscosity.

Polymer viscoelasticity and glass transition (T_g): Stress-strain behavior, Stress relaxation, Maxwell-Voigt mechanical models, glass and melting transition, thermodynamic aspects of T_g, determination of T_g (calorimetry, dynamic mechanical analysis), factors affecting T_g.

Networks, gels and rubber elasticity: Gel point, rubbery elastic states of polymers, thermodynamics of polymer elasticity-equation of state, ideal elastomers.

Crystalline state of polymers: Polymer Crystallization, thermodynamics and kinetics of crystallizations, semi-crystalline structures, experimental methods.

Applications and emerging technologies: Conducting and semi-conducting polymers in organic electronics, liquid crystalline polymers, self-assembly, Merrifield resins, polymer nanocomposites, plasticizers, antioxidant, adhesives.

Suggested Readings **:**

- *Polymer Chemistry*,P. C. Hiemenz and T.P. Lodge, 2nd Edition, CRC Press, 2007.
- *Introduction to Physical Polymer Science*, L.H. Sperling, Wiley-Interscience, 2006.
- *Principles of Polymer Chemistry*, P.J. Flory, Cornell University Press, 1953.

CHM 633: Quantum Chemistry (4)

Prerequisites: *CHM 322/642 or PHY 303 or equivalent*

Review of the postulates of quantum mechanics. Introduction to Hilbert spaces and bra-ket algebra. Symmetry and conservation laws, Ehrenfest theorem and quantum-classical correspondence. Electron spin angular momentum, spin operators and eigenfunctions. Addition of angular momenta, spin-orbit coupling.

Many-electron systems, antisymmetry principle, Slater determinant wave functions, Pauli exclusion principle. The Independent particle approximation to many-electron atoms, atomic term symbols for ground and excited states. Molecular Hamiltonian, Born-Oppenheimer approximation.

The independent particle approximation applied to molecules, MO treatment of H2+ molecular ion, LCAO approach to polyatomic molecules, Huckel and extended Huckel theories and simple applications.

Electron-electron correlations, Hartree-Fock theory and the SCF method, Koopmans' theorem, Brillouin's theorem, restricted and unrestricted approaches, Gaussian basis sets and pplications to simple molecules.

Correlation energy, a survey of post-HF and semi-empirical methods. Introduction to density-functional theory, Hohenberg-Kohn theorems, Kohn-Sham equations, exchange-correlation functionals and some applications.

Suggested Readings **:**

- Levine, I., *Quantum Chemistry*, Ed. 6th, Pearson Press, **2009**.
- McQuarrie, D. A., *Quantum Chemistry*, Ed. 2nd, University Science Books, **2008**.
- Atkins, P. W., Friedman, R. S., *Molecular Quantum Mechanics*, Oxford University Press, **2008**.
- Szabo, A., Ostlund, N. S., *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Dover, **1989**.

CHM 635: Mathematical Methods for Chemists (4)

Prerequisites: *MTH 101, MTH 102, MTH 201, MTH 202*

***Learning Objectives*:**

The main objective of this course is to provide students of chemistry the necessary skills and confidence to apply simple ideas and methods in mathematics.

***Course Contents*:**

Differentiation and integration; seried and limits, vector calculus; linear algebra and vector spaces; determinants, matrices and eigenvalue problems; curvilinear coordinates; functions of a complex variable; ordinary and partial differential equations; Fourier series, integral transforms; introduction to probability and statistics.

***Suggested Readings* :**

- McQuarrie, D. A., *Mathematical methods for scientists and engineers*, University Science Books, **2003**.
- Arfken, G., Weber, H., and Harris, F., *Mathematical methods for physicists*, Academic Press, Ed. 7th, **2012**.
- Boas, M. L, *Mathematical methods for the physical sciences*, Kaye Pace, Ed. 3rd, **2006**.
- Matthews, J., and Walker, R. L., *Mathematical methods of physics*, Addison Wesley Longman, Ed. 2nd, **1971**.

CHM 637: Chemistry and Physics of Materials (4)

Prerequisites: *CHM 222, CHM 322/642 or PHY 303*

Learning Objectives**:**

The prime objective of this course is to understand structure and properties of advanced functional materials in bulk and in nanodimension. Applications of materials in the filed of energy, bio-imaging and opto-electronics is also one of the main learning objectives of this course.

Course Contents**:**

Structure and Bonding in Materials: Ideal structures, types of interactions and bonding, experimental determination of structure, defects and disorder in solids.

Review of Basic Concepts: Quantum mechanics, thermodynamics and statistical mechanics, electricity and magnetism, interaction of radiation with matter.

Properties of Materials: Electronic properties of solids, transport properties, thermal conductivity, lattice dynamics and structural phase transitions, absortion and scattering of radiation by crystals, electro-optic and photovoltaic effects, and elastic phenomena.

Structure and Properties at the Nano-scale: Optical, electronic and structural properties of confined systems, principles of electron microscopy and other experimental tools for nano-science.

Surface Science: Introduction to surface structure, electronic states, adsorption, reactivity of surfaces, surface free energy and stress.

Functional Materials

Suggested Readings **:**

- The Physics and Chemistry of Materials – Joel I. Gersten, Fredrick W. Smith.
- Introduction to Nano-science and Nano-technology – Massimiliano DiVentra, *et al.*
- Solid State Physics – Guiseppe Grosso and Guiseppe Pastori Parravicini.

CHM 641: Symmetry and Group Theory (4)

Prerequisites: *CHM 102*

*Molecular Symmetry**:*** Symmetry elements and symmetry operations, definition of group and its characteristics, subgroups, classes, similarity transformation. Products of symmetry operations, relations between symmetry elements and operations, symmetry elements and optical activity, classes of symmetry operations, Conventions regarding coordinate system and axes, point group and classification, degenerate point groups, examples, Some properties of matrices, representation of groups, reducible and irreducible representations, the great orthogonality theorem, character tables, position vector and base vector as basis for representation, Wave functions as basis for irreducible representations (p- and d-orbitals) direct product, vanishing integral.

Symmetry adopted linear combinations: Projection operators and some examples, e.g. π-orbitals for the cyclopropenyl group etc.

Applications:

Symmetry Aspects of Molecular Orbital Theory: General Principles, symmetry factoring of secular equations, carbocyclic systems, more general cases of LCAO-MO bonding, examples, Huckel Molecular orbital theory systems, e.g., π-systems and conjugated π-systems, benzene and naphthalene, delocalization energies, resonance energies and aromaticity, the bond order (p) and free valence number (F), three centre bonding.

Hybrid orbitals and Molecular orbitals: transformation properties of atomic orbitals, hybridization schemes for bonding and for π -bonding, hybrid orbitals as LCAO, examples, MO theory for AB_n, molecular orbital theory for regular octahedral and tetrahedral molecules.

Molecular Vibrations: Normal Mode analyses *via* IR and Raman spectroscopy. Selection rules, spectral transition probability, vibronic coupling, electronic spectra of inorganic complexes and ions. Splitting of one electron level in an octahedral and tetrahedral environment.

***Suggested Books*:**

- *Chemical Applications of Group Theory*, F. A. Cotton, 3rd edition, Wiley InterScience, New York, **1990**.
- *Molecular Symmetry and Group Theory*, R. L. Carter, John Wiley & Sons, India, **2004**, **2005**.
- *Molecular Symmetry and Group Theory*, A. Vincent, 2nd Edition, John Wiley & Sons Ltd, England, **2001**.
- *Symmetry and Spectroscopy of Molecules*, K. Veera Reddy, New Age International (P) Ltd, India, **2010**.
- *Group Theory and Chemistry*, D. M. Bishop, Dover Publications, New York, **1993**.

CHM 642: Principles of Quantum Chemistry (4)

Prerequisites: *MTH 101, PHY 101, CHM 101, MTH 102, PHY 102, MTH 201, PHY 201 or their equivalent* **Not allowed for Physics majors**

Review of basic concepts of quantum theory: wave-particle duality and de Broglie wavelengths, uncertainty principle, superposition and state of a quantum system.

Mathematical background: Operators in quantum mechanics and their properties, eigenvalues and eigenfunctions, commutation relations, unitary transformations and change of basis. Matrix representation of operators.

Postulates of quantum mechanics: States and wavefunctions, observables and the measurement hypothesis, Born interpretation of wavefunction, time evolution of states and the Schrodinger equation, stationary states, compatible observables and the generalized uncertainty principle.

One-dimensional problems: Particle in a well and transmission through a barrier. Probability currents and the equation of continuity. Two and three-dimensional potential wells and degeneracy. Applications to conjugated molecules and other one-dimensional systems. Linear harmonic oscillator – ladder operator method, parity of harmonic oscillator eigenfunctions. Rigid rotor problem, angular momentum, angular momentum eigenvalues and eigenfunctions.

The hydrogen atom: Atomic orbitals – radial and angular wavefunctions and distributions, electron-spin and spin operators. Virial theorem and application to hydrogen atom and other problems. Hydrogen-like atoms.

Atoms in external fields: Zeeman and Stark effect.

Approximation methods: Time-independent perturbation theory – Anharmonic oscillator, He atom, H^{2+} molecular ion. Variational theorem - He atom, H^{2+} molecule and the LCAO approach.

***Suggested Books*:**

- Levine, I., *Quantum Chemistry*, Ed. 6th, Pearson Press, **2009**.
- McQuarrie, D. A., *Quantum Chemistry*, Ed. 2nd, University Science Books, **2008**.
- Zettili, N., *Quantum* Mechanics, Ed. 2nd, John Wiley, **2009**.
- Atkins, P. W., Friedman, R. S., *Molecular Quantum Mechanics*, Oxford University Press, **2008**.

CHM 651: Chemical Dynamics and Non-Adiabatic Interactions (4)

Prerequisites: *CHM 322/642 or PHY 303*

The Born-Oppenheimer Approach – The Time Independent Framework: (a) The Adiabatic Representation; (b) The Diabatic Representation

Mathematical Introduction: (a) The Hilbert Space and the Curl-Div Equations; (b) First Order Differential Equations along contours; (c) Abelian and non-Abelian Systems.

The Adiabatic-Diabatic Transformation (ADT). On the Single-valuedness of the newly formed Diabatic Potentials and the Quantization of the Born-Oppenheimer (BO) non-adiabatic coupling (NAC) matrix. Singularities, Poles and Seams characterizing the BO-NAC terms.

Molecular Fields as formed by Lorentz Wave-Equations.

The Jahn-Teller Model, The Renner-Teller model, the mixed Jahn-Teller/Renner-Teller model. The Privileged ADT phase and the corresponding Topological (Berry/Longuet-Higgins) phase.

The Extended Born-Oppenheimer Equation including Symmetry

The Born-Oppenheimer Approach – The Time Dependent Framework (emphasizing Field-dependent non-Adiabatic Coupling terms).

The interaction between molecular systems and electromagnetic fields: (a) The Classical treatment of the field (b) The Quantum treatment of the Field (based on Fock states). If time allows various subjects related to Quantum Reactive Scattering Theory will be introduced. Among other things the concept of arrangement channels and decoupling of arrangement channels employing Absorbing Boundary conditions will be discussed.

Suggested Readings **:**

- M. Baer and C-Y. Ng, (eds), State-Selected and State-to-State Ion-Molecule Reaction Dynamics. Ser. Advances of Chemical Physics, Vol. 82, Part 2, John Wiley, Hoboken, N.J. (1992)
- M. Baer and G.D. Billing (eds), The Role of Degenerate States in Chemistry, Ser. Advances of Chemical Physics, Vol. 124; John Wiley, Hoboken, N.J. (2002)
- W. Domcke, D.R. Yarkony and H. Koeppel, Conical Intersections, Advances Series in Physical Chemistry Vol. 15 (World Scientific, Hong-Kong (2004).
- Farad. Discussions, Non-Adiabatic Effects in Chemical Dynamics, Vol. 127 (R.S.C.), University Oxford, (2004)
- M. Baer, Beyond Born-Oppenheimer: Electronic Nonadiabatic Coupling Terms and Conical Intersections, Wiley Interscience, Hoboken, N.J., (2006).
- G.C. Schatz and M. A. Ratner, Quantum Mechanics in Chemistry, Prentice-Hall, Englwood Cliffs (1993)
- J.D. Jackson, Classical Electrodynamics, 2nd Edition, John Wiley, New York (1975)
- J. Z. H. Zhang, Theory and Application of Quantum Molecular Dynamics, World Scientific, Hong-Kong (1999)