CHEMISTRY

I Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits (AL/3)
CHM 101	General Chemistry	3	1	4.5	0	0	8.5	4	O to F	3

II Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits (AL/3)
CHM 112	Basic Organic Chemistry-I	3	1	4.5	0	0	8.5	4	O to F	3
CHM 114	Chemistry Laboratory- I	0	0	1	3	0	4	3	O to F	1

III Semester

	Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits (AL/3)
Chemistry											
DC	CHM211	Basic Organic Chemistry-II	3	1	4.5	0	0	8.5	4	O to F	3
	CHM221	Basic Physical Chemistry	3	1	4.5	0	0	8.5	4	O to F	3
	CHM223	Chemistry Laboratory II	0	0	1	3	0	4	3	O to F	1
MD	Nil										

IV Semester

	Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits (AL/3)
Chemistry											
DC	CHM204	Basic Inorganic Chemistry	3	1	4.5	0	0	8.5	4	O to F	3
	CHM206	Chemistry Laboratory III	0	0	1	3	0	4	3	O to F	1
	CHM222	Classical Thermodynamics	3	1	4.5	0	0	8.5	4	O to F	3
MD	Nil										

DC: Departmental Compulsory Course; **MD:** Mandatory Course from Other Department; **RD:** Recommended Course from Other Department

V Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits
CHM 301	Symmetry and Group Theory	3	0	7.5	0	0	10.5	3	O to F	4
CHM 311	Organic Chemistry I	3	0	7.5	0	0	10.5	3	O to F	4
CHM 313	Organic Chemistry Laboratory	0	0	2	6	0	8	6	O to F	3
CHM 321	Physical Chemistry of Solutions	3	0	7.5	0	0	10.5	3	O to F	4
CHM 325	Mathematical Methods for Chemists	3	0	7.5	0	0	10.5	3	O to F	4
*** ***	Department/Open Elective I	3	0	4.5/7.5	0	0	7.5/10.5	3	O to F	3/4
Total Credits		**15**	**0**	**36.5/39.5**	**6**	**0**	**57.5/60.5**	**21**		**22/23**

VI Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits
CHM 302	Chemistry of Transition Metals	3	0	7.5	0	0	10.5	3	O to F	4
CHM 312	Organic Chemistry II	3	0	7.5	0	0	10.5	3	O to F	4
CHM 314	Quantitative Methods in Chemistry	3	0	7.5	0	0	10.5	3	O to F	4
CHM 322	Principles of Quantum Chemistry	3	0	7.5	0	0	10.5	3	O to F	4
CHM ***	Departmental Elective II	3	0	7.5	0	0	10.5	3	O to F	4
*** ***	Open Elective II	3	0	4.5/7.5	0	0	7.5/10.5	3	O to F	3/4
Total Credits		**18**	**0**	**42/45**	**0**	**0**	**60/63**	**18**		**23/24**

VII Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits

CHM 401	Main Group Chemistry	3	0	7.5	0	0	10.5	3	O to F	4
CHM 403	Inorganic Chemistry Laboratory	0	0	2	6	0	8	6	O to F	3
CHM 411	Physical Organic Chemistry	3	0	7.5	0	0	10.5	3	O to F	4
CHM 421	Statistical Mechanics	3	0	7.5	0	0	10.5	3	O to F	4
CHM ***	Departmental Elective III	3	0	7.5	0	0	10.5	3	O to F	4
*** ***	Open Elective III	3	0	4.5/7.5	0	0	7.5/10.5	3	O to F	3/4
Total Credits		**15**	**0**	**36.5/39.5**	**6**	**0**	**57.5/60.5**	**21**		**22/23**

VIII Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits
CHM 402	Applications of Modern Physical Methods	3	0	7.5	0	0	10.5	3	O to F	4
CHM 416	Spectroscopy and Its Application in Organic Molecules	3	0	7.5	0	0	10.5	3	O to F	4
CHM 422	Molecular Spectroscopy	3	0	7.5	0	0	10.5	3	O to F	4
CHM 426	Physical Chemistry Laboratory	0	0	2	6	0	8	6	O to F	3
CHM ***	Departmental Elective IV	3	0	7.5	0	0	10.5	3	O to F	4
*** ***	Open Elective IV	3	0	4.5/7.5	0	0	7.5/10.5	3	O to F	3/4
Total Credits		**15**	**0**	**36.5/39.5**	**6**	**0**	**57.5/60.5**	**21**		**22/23**

IX Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits
CHM 501	MS Thesis	-	-	-	-	-	25	-	O to F	10
CHM ***	Departmental Elective V/ Research Credit	3	0	7.5	0	0	10.5	3	O to F	4
CHM ***	Departmental Elective VI/ Research Credit	3	0	7.5	0	0	10.5	3	O to F	4
HSS 503	Law Relating to Intellectual Property and Patents	1	0	2.5	0	0	3.5	1	S/X	1
Total Credits		**7**	**0**	**17.5**	**0**	**0**	**49.5**	**7**		**9**

X Semester

Course No.	Course Title	Lec Hr	Tut Hr	SS Hr	Lab Hr	DS Hr	AL	TC Hr	Grading System	Credits
CHM 501	MS Thesis	-	-	-	-	-	45	-	O to F	18
Total Credits		**-**	**-**	**-**	**-**	**-**	**45**	**-**	**-**	**18**

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 fundamental principles of chemistry. This includes, the atomic structure, periodicity of elemental properties, chemical bonding, acids and bases and radioactivity.

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 hetero diatomic molecules, concept of frontier orbitals. HCP and CCP structures of solids, radius ratio rules, Simple cubic solids & Lattice Energy (Born-Haber cycle).

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.

Radioactivity and Nuclear Chemistry: The nature of radioactive radiation, 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

1. Lee, J.D., *Concise Inorganic Chemistry*, 5th Ed., Blackwell Publishing,

2006.
2. Cotton, F.A., Wilkinson, G., Gaus, P. L., *Basic Inorganic Chemistry*, 3rd Ed., John Wiley and Sons Press, **1995**.
3. Atkins, P., et al., *Shriver and Atkins Inorganic Chemistry,* 4th Ed., Oxford University Press, **2006**.
4. Kotz J. C., Treichel, P. M., Townsend, J., *Chemistry and Chemical Reactivity,* 8th Ed., Brooks Cole, **2011**.

CHM 112: Basic Organic Chemistry (3)

Learning Objectives

This is an introductory course for the first year BSMS students. It familiarizes them to the basic concepts in the Chemistry of Organic molecules such as cause of stability and reactivity of Organic compounds, and the major pathways taken by Organic compounds during reactions.

Course Contents

Chemistry of Carbon: Hybridization of atomic orbitals, C-C single, double and triple bonds, bonding with O and N, delocalization and conjugation (allyl, butadiene orbital diagrams), HOMO/LUMO concept, aromaticity and Frost diagrams.

Electronic effects: Dipole moment, polarizability, inductive effects, resonance, hyper-conjugation.

Acids and Bases: Concepts of pH, pK_a, pK_b as applied to organic compounds

Stereochemistry of Organic Molecules: Fischer, Newman, Sawhorse, 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.

Reactive Intermediates: Introduction to structure, formation, stability and reactions of carbocations, carbanions, free radicals, radical anions, radical cations, arynes, carbenes and nitrenes.

Introduction to Organic Reactions: Electrophilic and radical additions to alkenes, electrophilic and nucleophilic aromatic substitutions, nucleophilic aliphatic substitutions: S_N1, S_N2, S_Ni reactions, neighboring group participation, elimination reactions: E_1, E_2, and E_{1cB} reactions, nucleophilic addition reactions.

Suggested Books

1. Clayden, J. et al., *Organic Chemistry*, 2nd Ed., Oxford University Press, **2001**.
2. Hornback, J. M., *Organic Chemistry*, 2nd Ed., Cengage Learning, **2006**.
3. Solomons, T. W. G. and Fryhle, C. B., *Organic Chemistry*, 9th Ed. John Wiley and Sons, **2007**.
4. Morrison, R. M. and Boyd, R. N., *Organic Chemistry*, 6th Ed., Pearson Education, **2008**.
5. Sykes, P. A., *A guide book to mechanism in organic chemistry*, 6th Ed., Pearson India, **2008**.

CHM 114: 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 211: Basic Organic Chemistry – II (3)

Learning Objectives

This course intends to provide a strong foundation to the Chemistry pre-majors on the stereo-chemical aspects of organic molecules. It also delves into the various rearrangements that organic compounds undergo, and details the mechanisms involved in such rearrangements. In the later part of the course, Organic Chemistry of relevance to Biology is introduced.

Course Contents

Stereochemistry: Conformational analysis, conformation of acyclic, cyclic, fused and bridged systems, Strain in cyclic and acyclic molecules including allylic strain ($A^{1,2}$ and $A^{1,3}$), Dynamic stereochemistry: Conformation and reactivity, Curtin-Hammett principle.

Rearrangement and Fragmentation 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), Fragmentation reactions.

Introduction to Biological Organic Chemistry: Basic structure and reactivity of amino acids, nucleic acids, carbohydrates, and lipids, Functional groups and their modular design in biomolecules, Importance of non-bonding interactions and their role in biological reactions: ionic interactions, hydrophobic interactions, van der Waals interactions, hydrogen bonding.

Suggested Books

1. Clayden, J. et al., *Organic Chemistry*, 2nd Ed., Oxford University Press, **2001**.
2. Hornback, J. M., *Organic Chemistry*, 2nd Ed., Cengage Learning, **2006**.
3. Morrison, R. M. and Boyd, R. N., *Organic Chemistry*, 6th Ed., Pearson Education, **2008**.
4. Eliel, E. L., Wilen, S. H., Doyle, M. P., *Basic Organic Stereochemistry*, 1st Ed., John Wiley and Sons, **2001**.
5. Smith, M. B. and March, J., *Advanced Organic Chemistry*, 6th Ed., John Wiley and Sons, **2007**.
6. Carey, F. A, Sundberg, R. J., *Advanced Organic Chemistry*, Parts A and B, Springer, **2007**.

CHM 221: Basic Physical Chemistry (3)

Learning Objectives

This course deals with concepts related to properties of fluids, conductance and preliminary introduction to chemical kinetics. This course is a basic course for all students interested in Chemistry and the concepts taught here would be required for most of the courses that follow in this stream.

Course Contents

Properties of the Gaseous State: Gas Laws, equation of states, real gases, 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, virial expansions.

Viscosity of fluids, surface tension of liquids, capillary rise and basic applications.

Conductance: Mechanism of electrolysis and Faraday's law, strong and weak electrolytes (review of molarity, molality, normality), conductance, electrolytic conductance, ionic conductance, conductometric titration, estimation of solubility product.

Chemical Kinetics: Rate laws, order and molecularity, determination of order of a reaction, kinetics of zero, first and second order reactions, parallel, reversible and consecutive reactions. Concept of steady state and its application.

***Suggested Books*:**

1. Levine, I., *Physical Chemistry*, 6^{th} Ed., McGraw Hill, **2009**.
2. Atkins, P.W. and de Paula, J., *Physical Chemistry*, 9^{th} Ed., Oxford Press, **2009**.
3. Castellan, G.W., *Physical Chemistry*, 3^{rd} Ed., Narosa Publishing House, **2004**.

CHM 223: Chemistry Laboratory – II (1)

Learning Objectives

Students will be introduced to basic experiments in physical chemistry involving pH-metry, conductometry, chemical kinetics, etc.

Suggested Experiments

- Kinetics of the iodide-hydrogen peroxide clock reaction.
- First order kinetics – Acid hydrolysis of methyl acetate at different temperatures at a given concentrations of [H^+] ions.
- First order kinetics – Acid hydrolysis of methyl acetate at different concentrations of [H^+] ions at a given temperature.
- Kinetics of saponification of ethyl acetate using conductometry.
- Determination of acid dissociation constant (pK_a) of (A) polybasic acid (H_3PO_4) (B) Monobasic Acid (CH_3COOH).
- Acidic and basic dissociation constants of glycine and its isoelectric point.
- Determination of dissociation constant and equivalent conductance at infinite dilution of weak electrolyte (acetic acid) using conductometry.
- 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.
- Verification of Lambert-Beer law using colorimetry.

CHM 204: Basic Inorganic Chemistry (3)

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 (ionic & covalent) in inorganic chemistry, Chemical forces, Bent's rule, Application of molecular orbital theory to triatomic linear molecules (localized and delocalized orbitals), Walsh diagrams.

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

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 and hyper-valency.

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.

***Suggested Books*:**

1. Atkins, P., et al., *Shriver and Atkins Inorganic Chemistry*, 4th Ed., Oxford University Press, **2006**.
2. Lee, J. D., *Concise Inorganic Chemistry*, 5th Ed., Blackwell Publishing, **2006**.
3. Cotton, F. A., Wilkinson, G., Gaus, P. L., *Basic Inorganic Chemistry*, 3rd Ed., John Wiley and Sons Press, **1995**.
4. Douglas, B., McDaniel, D., Alexander, J., *Concepts and Models of Inorganic Chemistry*, 3rd Ed. Wiley India (P.) Ltd., India, **2010**.

CHM 206: Chemistry Laboratory – III (1)

Learning Objectives

To learn practical experimental execution of basic synthetic and analytical aspects in inorganic chemistry.

Suggested Experiments

- Qualitative analysis of inorganic salts.
- Recycling of aluminium: Preparation of potash alum from waste aluminium
- Preparation of $[Ni(NH_3)_6]^{2+}$ and estimation of nickel by gravimetric method
- Synthesis of tris(acetylacetonato) cobalt complex
- Synthesis of copper thiourea complex
- Standardization of a given solution of $KMnO_4$ through redox-titration
- Determination of acid-neutralizing power of a commercial antacid through acid-base titration
- Determination of Ca in milk powder through EDTA complexometry
- Estimation of iodine content in iodized common salt using iodometry
- Estimation of Cu in a copper complex (e.g., copper thiourea complex)
- Titration of a mixture of NaOH (aq) and Na_2CO_3 (aq)
- Photochemical reduction of ferric oxalate and its use in cyanotype/blueprinting

CHM 222: Classical Thermodynamics (3)

Learning Objectives

The concepts related to a fundamental understanding of thermodynamics will be presented. In this course, laws of thermodynamics, equilibrium and phase rule will be discussed. This course is not only crucial for chemistry but for other branches of sciences as well such as physics, earth science, biology and even engineering.

Course Contents

Zeroth law of thermodynamics: Equilibrium and concept of temperature.

First Law of thermodynamics: State and path functions, extensive and intensive properties, equation of state, work, heat, internal energy, heat capacity and concept of enthalpy.

Second law of thermodynamics: Reversible and irreversible process, heat engines, Carnot cycle, statements of the second law, concept of entropy, free energy, criteria for equilibrium and stability.

Third law of thermodynamics: Concept of the absolute zero temperature and Nernst heat theorem.

Equilibrium thermodynamics: Chemical potential, Gibbs-Duhem equations, phase equilibrium, Clapeyron equation, Claussius-Clayperon equation, phase rule, phase diagram, phase transitions in one-component and multi-component systems, chemical equilibrium, interrelations between K_p, K_c and K_x, effect of temperature (van't Hoff equation) and pressure on equilibrium constant.

Suggested Books

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

CHM 301/641: Symmetry and Group Theory (4)

Prerequisites (Desirable)*: CHM 101, CHM 204*

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.

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

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

CHM 311: Organic Chemistry – I (4)

***Prerequisites (Desirable)**: CHM 101, CHM 211*

Learning Objectives

This course introduces the Chemistry majors to the stereoelectronic effects involved in chemical reactions. Then it discusses the different reagents available to undertake oxidation and reduction of organic compounds and finally, it discusses the synthesis and properties of compounds that contain heteroatoms (N, S, O etc.).

Course Contents

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, Stereoselective reactions of cyclic molecules.

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.

Suggested Books

1. Clayden, J. et al., *Organic Chemistry*, 2nd Ed., Oxford University Press, **2001**.
2. Hornback, J. M., *Organic Chemistry*, 2nd Ed., Cengage Learning, **2006**.
3. Eliel, E. L., Wilen, S. H., Doyle, M. P., *Basic Organic Stereochemistry*, 1st Ed., John Wiley and Sons, **2001**.

4. Smith, M. B. and March, J., *Advanced Organic Chemistry*, 6th Ed., John Wiley and Sons, **2007**.
5. Carey, F. A, Sundberg, R. J., *Advanced Organic Chemistry*, Parts A and B, Springer, **2007**.
6. Anslyn, E. V. and Dougherty, D. A., *Modern Physical Organic Chemistry*, University Science Books, **2005**.

CHM 313: Organic Chemistry Laboratory (3)

Prerequisites (Desirable)*: CHM 211*

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-, region- 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 321: Physical Chemistry of Solutions (4)

Prerequisites (Desirable)*: CHM 213, CHM 222 (or equivalent)*

Learning Objectives

Concepts related to ideal and non-ideal solutions, phase equilibrium of binary mixtures, basic electrochemistry and rate theories involved in chemical kinetics would be discussed. This course is crucial for chemistry students since the topics covered are necessary for all branches of chemists.

Course Contents

Ideal and non-ideal solutions: Raoult's law and Henry's law, colligative properties, activity and review of thermodynamic equilibrium.

Ionic solutions: 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.

Rate theories: Arrhenius equation, Lindemann hypothesis, collision rate theory, transition state theory, enzyme kinetics and catalysis.

Suggested Books

1. Atkins, P. W., de Paula, J., *Physical Chemistry*, 9th Ed., Oxford Press, **2009**.
2. Castellan, G.W., *Physical Chemistry*, 3rd Ed., Narosa Publishing House, **2004**.
3. Levine, I., *Physical Chemistry*, 6th Ed., McGraw Hill, **2009**.

4. Laidler, K.J., *Chemical Kinetics,* 3rd Ed., Pearson Education India, **2003**.
5. Glasstone, S., *An Introduction to Electrochemistry,* original **1942**, reprint 2006.
6. Bard, A.J. and Faulkner, L.R., *Electrochemical Methods: Fundamentals and Applications*, 2nd Ed., John Wiley & Sons, **2001**.
7. Bockris, J.O'M, Reddy, A.K.N, *Modern Electrochemistry Ionics: Volume 1*, 2nd Ed., Plenum Press, **1998**.

CHM 325/635: Mathematical Methods for Chemists (4)

Prerequisites (Desirable): *MTH 101, MTH 102*

Learning Objectives

This is a compulsory course for 3rd year BS-MS, integrated Ph.D. Chemistry major students and is an elective for Ph.D. students in the Chemistry department. 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. This course is essential, as the methods introduced here would be applied in various courses taught in the forthcoming semesters.

Course Contents

Linear algebra: Vector spaces and matrices, determinants, inverse of a matrix, eigenvalue problems, coordinate transformation, Jacobian, curvilinear coordinates, eigenvalues and eigenvectors.

Complex numbers and variables: Functions of a complex variable, Complex algebra, functions of complex variables, Cauchy-Riemann conditions, analytic functions, Cauchy's integral theorem, contour integrals and the Cauchy integral formula, Laurent series.

Multivariable calculus: Functions of two or more variables, limits and continuity, partial derivatives, gradient, directional derivatives, maxima, minima and saddle points, Lagrange multipliers, line integrals, surface integrals, Green's theorem.

Vector calculus: Gradient, divergence, continuity equation, curl, Stokes' and Gauss' theorems.

Integral transforms: Fourier series, Fourier and Laplace transforms and their applications.

Ordinary differential equations: First order equations and their applications. Separation of variables, equations reducible to separable form. Second order linear differential equations: homogeneous with constant coefficients.

Suggested Books

1. McQuarrie, D. A., *Mathematical methods for scientists and engineers*, University Science Books, **2003**.
2. Arfken, G., Weber, H., and Harris, F., *Mathematical methods for physicists*, Academic Press, 7th Ed., **2012**.
3. Boas, M. L., *Mathematical methods for the physical sciences*, Kaye Pace, 3rd Ed., **2006**.

CHM 331: Fundamentals of Supramolecular Chemistry (4)

Prerequisites (Desirable): *CHM 204*

Learning Objectives

The objective of this interdisciplinary course is to learn the fundamental principles of molecular recognition and supramolecular chemistry. The focus will be to (i) identify different types of non-covalent interactions, (ii) interpret the thermodynamics of host-guest interactions, (iii) discuss the molecular recognition properties of common receptors, (iv) understand the principles of self-assembly, and (v) apply the principles of supramolecular chemistry to the design of functional architectures.

Course Contents

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. Coordination driven self-assemblies and molecular Cages.

Applications: Supramolecular Reactivity, Electronic devices (switches, wires and rectifiers) and non-linear optical materials.

Suggested Books

1. Steed, J. W. and Atwood, J. L., *Supramolecular Chemistry*, 2nd Ed., John Wiley and Sons, **2000**.
2. Lehn, J. -M., *Supramolecular Chemistry. Concepts and Perspectives*, Wiley VCH, **1995**.
3. Schneider, H.-J. and Yatsimirsky, A., *Principles and Methods in Supramolecular Chemistry*, John Wiley and Sons, **1999**.

CHM 343: Chemistry of Biological Systems (4)

Prerequisites (Desirable): *CHM 211*

Learning Objectives

In this course the Organic Chemistry of Life is discussed. Students will be exposed to the chemical entities involved in sustaining life, and the chemical reactions involved therein. The design of synthetic molecules to modulate the functions of biomolecules will also be introduced.

Course Contents

Chemistry of nucleic acids: Structure and properties of DNA and RNA bases, stability of DNA and RNA, chemical synthesis and reactivity of DNA, chemistry of DNA sequencing.

Amino acids: Structure and properties, solid phase peptide synthesis, protein sequencing methods, pKa and chemical reactivity of amino acid side chains, importance of sulfur in biological systems.

Proteins: secondary structure elements, Ramachandran plot, higher order protein structure, Enzymes and their interactions with substrate, basics of binding and kinetics, examples of mechanism based inhibitors. Chemistry of proteins coenzymes and cofactors: NADH, FAD, ascorbic acid, thiamine pyrophosphate, pyridoxal phosphate, SAM, acyl coenzyme A.

Carbohydrates: Mono-, di- and poly- saccharides, mutarotation, anomeric effect, reactions of carbohydrates, aminosugars, diabetes and artificial sweeteners, introduction to multivalency.

Fatty acids: Types and nomenclature, biosynthesis and oxidation pathways, membrane composition

Introduction to metabolism and bioenergetics, glycolysis, importance of ATP The biological periodic table, role of metal ion in biological functions, interaction of metals with proteins and nucleic acids

Concepts of Bioinorganic Chemistry: Oxygen carrier proteins - Structure and role of hemoglobin, myoglobin, hemerythrin, hemocyanin, Metal induced toxicity, chelation therapy, metals in medicine.

***Suggested Books*:**

1. Van Vranken, D. and Weiss, G., *Introduction to Bioorganic Chemistry and Chemical Biology*, Garland Science, **2013**.
2. Lippard, S. J. and Berg, J. M., *Principles of Bioinorganic Chemistry*, University Science Books, **1994**.
3. Clayden, J. et al., *Organic Chemistry*, 2nd Ed., Oxford University Press, **2001**
4. Berg, J., Tymoczko, J. and Stryer, L., *Biochemistry*, 5th Ed., W. H. Freeman, **2002**.

CHM 302: Chemistry of Transition Metals (4)

Prerequisites (Desirable): *CHM 204, CHM 301*

Learning Objectives

The main objective of this course is to understand the concepts of bonding, structure, property, and reactivity of transition metal complexes commonly involved in coordination chemistry, magnetism, organometallic systems, catalysis, and biological systems.

Course Contents

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. Nephelauxetic effect, Racah Parameters, Irving William series, Thermodynamic aspects of coordination complexes, Stereochemistry of non-rigid and fluxional molecules. 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 and properties of lanthanides and actinides.

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. Magnetism of Lanthanide complexes. Spin-crossover complexes.

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

Suggested Books

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

Inorganic Chemistry, 3rd Ed. Wiley India (P.) Ltd., India, **2010**.
4. Cotton, F. A. et al., *Advanced Inorganic Chemistry*, 3rd Ed., John Wiley and Sons, **1995**.
5. Jolly, W. L., *Modern Inorganic Chemistry*, 2nd Ed., McGraw-Hill, NY, **1991**.
6. Shriver, D. F. and Atkins,P. W., *Inorganic Chemistry*, 3rd Ed. Oxford University Press, **1999**.
7. Day, M. C., *Theoretical Inorganic Chemistry,* 2nd Ed., East-West Press, India, **2007**.
8. Mingos, D. M. P., *Essential Trends in Inorganic Chemistry*, OUP, New York **2010**.
9. Wulfsberg, G., *Inorganic Chemistry*, Viva Books P. Ltd, India, **2010**.
10. Li, W.-K., Zhou, G.-D. and Mak, T. C. W., *Advanced Structural Inorganic Chemistry,* IUCr Monograph, OUP, New York, **2008**.

CHM 312: Organic Chemistry – II (4)

Prerequisites (Desirable): *CHM 311*

Learning Objectives

This course familiarizes Chemistry students to a variety of chemical reactions and how Chemical synthesis is designed and planned. It aims to provide a strong emphasis on reactions and reagents employed to undertake enantioselective chemical transformations.

Course Contents

Carbon-Carbon Bond Forming Reactions: Bond formation via enolate, enamine and imine chemistry, Grignard, cuprate and other conjugate reactions, Olefination (Wittig, HWE, Julia and Peterson) and cyclopropanation reactions, and controlling double bond geometry, Radical reactions, Other classes (Baylis-Hillman reaction etc).

Organo-main group chemistry: Sulfur-ylids, organo-silicon, boron, and tin based reagents.

Enantioselective Reactions: Principles of enantioselective reactions, Resolution of racemic compounds and biodiscrimination of stereoisomers (amino acids, thalidomide, DOPA, nicotine, morphine), 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*:**

1. Clayden, J. et al., *Organic Chemistry*, 2nd Ed., Oxford University Press, **2001**.
2. Carruthers, W. and Coldham, I., *Some Modern Methods of Organic Synthesis*, Cambridge University Press, **2004**.
3. Smith, M. B., *Organic Synthesis*, McGraw-Hill, **2001**.
4. Smith, M. B. and March, J., *Advanced Organic Chemistry*, 6th Ed., John Wiley and Sons, **2007**.
5. Warren, S., *Organic Synthesis: The Disconnection Approach*, Wiley, **1983**.
6. Carey, F. A. and Sundberg, R. J., *Advanced Organic Chemistry*, Part A and B, Springer, **2007**.

CHM 314: Quantitative Methods in Chemistry (4)

Prerequisites (Desirable): *CHM 325*

Learning Objectives

This course aims to sensitize students towards appropriate scientific reporting of the data, and use of statistics for testing hypothesis. It also emphasizes the reproducibility of experiments and the sources of "errors" during repetitions of experiments. In the later part, it deals with the principles of separation techniques employed on synthetic chemicals and biomolecules.

Course Contents

Calculations used in Chemistry: Chemical Stoichiometry, Molarity, Molality, etc.

Concepts of sampling and experimental errors in chemical analysis: Gross errors and their sources, statistical treatment and evaluation of data, Standard deviation (and other metrics) for quantifying reproducibility of data and their calculation, Scientific reporting of data, Confidence levels and confidence intervals, statistical aids in hypothesis testing, Analysis of variance, Linear regression, Software-based data analysis

Preparing samples for analysis: primary, secondary standard etc., Classical methods of analysis: Gravimetric, Volumetric, Titrimetric, Potentiometric methods.

Separation techniques used in modern chemistry: Concept of theoretical plate and plate heights in chromatographic separations, Gas chromatography, HPLC, Supercritical fluid chromatography, Field flow fractionation and related methods. Solution and solid-phase reaction techniques.

Suggested Books

1. Skoog, D. A. et al., *Fundamentals of Analytical Chemistry*, 9th Ed., Cengage Learning, **2013**.
2. Clayden, J. et al., *Organic Chemistry*, 2nd Ed., Oxford University Press, **2001**.

CHM 322/642: Principles of Quantum Chemistry (4)

Prerequisites (Desirable): *CHM 101, PHY 101, PHY 102, CHM 325 or their equivalent.*

This course is not an elective for Physics majors.

Learning objectives

This is a compulsory course for 3rd year BS-MS major, integrated Ph.D. students and is an elective for Ph.D. students in the Chemistry department. It is an open-elective for 3rd and upper year students from other departments (except Physics) meeting the pre-requisites below. The course will aim at introducing fundamental principles of quantum chemistry and the mathematical framework necessary to solve problems relevant to atomic and molecular structure, and spectroscopy.

Course Contents

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.

Approximation methods: Time-independent perturbation theory and application to anharmonic oscillator, He atom.

***Suggested Books*:**

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

CHM 324: Physical Properties of Matter (4)

Prerequisites (Desirable): *CHM 213, CHM 222, CHM 321*

Learning objectives

This is a departmental elective course for 3rd year BS-MS chemistry major students and deals with the basic concepts of various intermolecular forces involved in chemical reactions. A thorough treatment of surface phenomena will enable students to understand the chemistry behind adsorption processes, properties of surface-active agents, and colloids. Finally, the course outlines the associated thermodynamics of polymer solutions and provides a better understanding of potential energy surfaces under the ambit of reaction dynamics.

Course Contents

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: The general equation for transport, diffusion, Fick's laws of diffusion, thermal conductivity.

Surface phenomena: Adsorption kinetics, Freundlich, Langmuir and BET isotherms.

Micelles and reverse micelles: Surfactants, types of surfactants, critical micelle concentration (CMC) and methods to estimate CMC, concept of Krafft temperature, thermodynamics of micellization, mass action model, pseudo-phase model.

Colloids: Lyophilic and lyophobic colloids, electrical double layer, electrokinetic effects, Hardy-Schulze law, soaps and detergents.

Thermodynamics of polymer solutions: Lattice model, elementary concepts of Flory-Huggins theory.

Reaction dynamics: Collision theory and potential energy surfaces.

Suggested Books

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

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

Prerequisites (Desirable): 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:

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.

Structure and Bonding in Solids: Factors governing formation of crystal structures, Kapustinskii's equation, Sanderson's Model, Mooser-Pearson plots, 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, Martensitic, order- disorder transitions.

Structure Property Correlation in Materials: Optical, Dielectric and Superconducting properties.

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).

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.

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. West, A. R., *Solid State Chemistry and its Applications*, 2^{nd} Ed. John Wiley & Sons, UK, **1999**.
2. Rohrer, G. S., *Structure and Bonding in Crystalline Materials*, 1^{st} Ed., Cambridge University Press, UK, **2001**.
3. Hammond, C., *Basics of Crystallography and Diffraction*, 4^{th} Ed., Oxford University Press, **2015**.
4. Stout, G. H. and Jensen, L. H., X-ray Structure determination: A practical guide, 2^{nd} Ed., Wiley-Blackwell, **1989**.

CHM 401/601: Main Group Chemistry (4)

Prerequisites (Desirable): *CHM 204, 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.

Representative chemistry of s- and p-blocks: alkali metals, boranes, carboranes, boron clusters, Wade's rules, *styx* numbers, 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.

Chemistry of heavier carbenes analogues: Push-pull carbenes, stable heavier carbene analogues (silicon, germanium, tin and lead): synthesis, characterization, structure and reactivity.

Suggested Books

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

CHM 403: Inorganic Chemistry Laboratory (3)

Prerequisites (Desirable): *CHM 204, CHM 301, CHM 302*

Learning Objectives

This is an advanced inorganic chemistry laboratory course. The objective is to learn synthetic methods of various inorganic compounds/complexes, study their properties via spectroscopic, electrochemical, and structural methods, and demonstrate some applications.

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 and acetylation reaction of ferrocene.
- Synthesis and electrochemistry of $[Ru(bpy)_3]^{2+}$.
- Preparation, recording and indexing of PXRD pattern of simple cubic solid.

CHM 411/611: Physical Organic Chemistry (4)

Prerequisites (Desirable): *CHM 311 and 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 Books

1. Isaacs, N. S., *Physical Organic Chemistry*, 2nd Ed., Longman Scientific & Technical, **1995**.
2. Deslongchamps, P., *Stereolectronic Effects in Organic Chemistry*, Pergamon, **1983**.
3. Carey, F. A. and Sundberg, R. J., *Advanced Organic Chemistry*, Part A and B, Springer, **2007**.
4. Turro, N. J., *Modern Molecular Photochemistry*, University Science Books, **1991**.
5. Anslyn, E. V. and Dougherty, D. A., *Modern Physical Organic Chemistry*, University Science Books, **2005**.
6. Woodward, R. B. and Hoffmann, R., *The Conservation of Orbital Symmetry*, Verlag Chemie, **1970**.
7. Lehr, R. E. and Marchand, A. P., *Orbital Symmetry: A Problem Solving Approach*, Academic Press, **1972**.

CHM 421/621: Statistical Mechanics (4)

Prerequisites (Desirable): *CHM 222, CHM 322, CHM 325*

Learning Objectives

This is a compulsory course for 4th year BS-MS major, integrated Ph.D. stduents and is an elective for Ph.D. students in the Chemistry department. It is an open-elective for 4th and upper year students from other departments meeting the pre-requisites below. 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 ofstatistical 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 Books

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

CHM 402/602: 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.

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.

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.

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

Mass Spectroscopy: Introduction and Applications to Isotopic systems.

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

Thermal methods of characterization: DSC and TGA.

Suggested Books

1. Gunther, H., *NMR Spectroscopy – An Introduction,* John Wiley, **1980**.
2. Brisdon, A. K., *Inorganic Spectroscopic Methods,* Oxford University Press, **2005**.

3. Iggo, J. A., *NMR Spectroscopy in Inorganic Chemistry,* Oxford University Press, **2011**.
4. *Parrish, R. V., NMR, NQR, EPR and Mossbauer spectroscopy in Inorganic Chemistry,* Ellis Horwood Limited, **1990**.
5. Drago, R. S., *Physical Methods in Inorganic Chemistry,* East-West Press Pvt. Ltd., **2012**.
6. Ebsworth, E. A. V., et al., *Structural Methods in Inorganic Chemistry,* 2nd Ed., CRC Press, **1991**.
7. Baird, A. J., and Faulkner, L. R., *Electrochemical methods – Fundamentals and applications,* Wiley, **1980**.
8. Scott, R. A. and Lukehart, C. M., *Applications of Physical Methods to Inorganic and Bioinorganic Chemistry,* Wiley, **2007**.

CHM 416/616: Spectroscopy and Its Application in Organic Molecules (4)

Prerequisites (Desirable): *CHM 311 and CHM 312*

Learning Objectives

This course emphasizes on the practical utilization of spectroscopic methods for determination and assignment of chemical structures of organic molecules. In addition to covering the basics of spectroscopic techniques such as FTIR, FT-NMR and Mass Spectrometry that are regularly used by Organic Chemists, practical examples of structure determination using these techniques are also discussed.

Course Contents

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 Books*:**

1. Pavia, D. L. et al., *Introduction to Spectroscopy*, 4th Ed., Brookes Cole, **2008**.
2. Gunther, H., *NMR spectroscopy: Basic principles, concepts, and applications in chemistry*, 3rd Ed., Wiley, **2013**.
3. Claridge, T., *High Resolution NMR Techniques in Organic Chemistry*, 2nd Ed. Elsevier, **2009**.
4. de Hoffmann, E. and Stroobant, V., *Mass Spectrometry, Principles and applications*, 3rd Ed., Wiley, **2007**.
5. Silverstein, R. M., Webster, F. X., Kiemle, D., *Spectrometric identification of organic compounds*, 7th Ed., Wiley, **2005**.

CHM 422/622: Molecular Spectroscopy (4)

Prerequisites (Desirable): *CHM 322, CHM 325, CHM 421, or their equivalent*

Learning Objectives

The course will aim to deliver (a) fundamentals of rotational, vibrational, Raman and electronic spectroscopy, (b) introduction to the theory behind these techniques and (c) applications of these techniques.

Course Contents:

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.

***Suggested Books*:**

1. Banwell, N., McCash, E. M., *Fundamentals of Molecular Spectroscopy*, Tata-McGraw Hill, **2007**.
2. Atkins, P. W., de Paula, J., *Physical Chemistry*, Ed. 9th, Oxford Press, **2009.**
3. Hollas, J.M., *Modern Spectroscopy*, 4th Ed. , John Wiley & Sons Ltd, **2004**.
4. Engel, T., *Quantum Chemistry and Spectroscopy,* Pearson Education, **2007**.
5. Wilson, E. B., Decius, J. C., and Cross, P. C., *Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra*, Dover, **1980**.
6. Harris, D. C., and Bertolucci, M. D., *Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy*, Dover, **1989**.

7. Steinfeld, J. I., *Molecules and Radiation: An Introduction to Modern Molecular Spectroscopy*, Ed. 2nd, Dover, **2005**.
8. Berry, R. S., Rice, S. A., Ross, J., *Physical Chemistry*, Ed. 2nd, Oxford Press, **2000**.

CHM 426: Physical Chemistry Laboratory (3)

Prerequisites (Desirable): *CHM 103, CHM 213, 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 603: Advanced Inorganic Chemistry – I (4)

Prerequisites (Desirable): *CHM 204, CHM 302*

Learning Objectives

To learn advanced and contemporary inorganic chemistry topics involving transition metal systems in detail.

Course Contents

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 bonds.

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 Books

1. Stochel, G., et al., *Bioinorganic Photochemistry*, Wiley, **2009**.
2. Lippard, S. J. and Berg, J. M., *Bioinorganic Chemistry*, University Science Books, **1994**.
3. Discussion on above mentioned topics with relevance to the recent literature.

CHM 604: Advanced Inorganic Chemistry – II (4)

Prerequisites (Desirable): *CHM 204, CHM 302, CHM 402*

Learning Objectives

To learn advanced and contemporary inorganic chemistry topics involving main-group elements in detail.

Course Contents

Basic concepts on non-transition elements chemistry: Chemical bonding, Structural elucidation by various spectroscopic methods.

Inorganic polymers: Borazines-, heterocyclophosphazenes-, siloxanes-, stannoxanes-derived polymers, sulfur-nitrogen polymers, phosphorus-nitrogen polymers, polysilane, poly-silazane, B-N polymers, precursors for ceramics and applications, phthalocyanins, conducting polymers, host guest interactions.

Interlocked macromolecules: Catenanes, rotaxanes, pseudorotaxanes.

Organometallic chemistry of non-transition elements: stability (thermodynamic and kinetic aspects), lability, general preparation methods, organometallic compounds of alkali, alkali earth metals and heavy main group elements: synthesis, stability, reactivity and structural aspects.

Organoelement compounds of boron, carbon, nitrogen, oxygen, fluorine groups: Synthesis, reactivity, stability, structural elucidation; structurally diverse π-cyclopentadienyl complexes of the main group elements; applications of organoelements in material, sensor, synthetic, bioinorganic (BNCT, thyroid hormones regulations, GPx-enzyme etc.) chemistry.

***Suggested Books*:**

1. Huheey, J. E., et al., *Inorganic Chemistry-Principles of Structure and Reactivity,* 4th Ed., Harper-Collins, **1993**.
2. Greenwood, N. N., and Earnshaw, A., *Chemistry of the Elements,* 1st Ed., Pergamon, Oxford, **1989**.
3. Elschenbroich*, C., Organometallics,* 3rd Ed., Wiley-VCH, **2006.**
4. Journal articles

CHM 605: Bioinorganic Chemistry (4)

Prerequisites (Desirable): *CHM 204, 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 Books*:**

1. Lippard, S. J., and Berg, J. M. , *Principles of Bioinorganic Chemistry*, University Science Books, **1994**.
2. Bertini, I., et al., *Bioinorganic Chemistry*, 1st Ed., **1998**.

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

Prerequisites (Desirable): *CHM 301*

Learning Objectives

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

Course Contents

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 Books*:**

1. Tareen, J. A. K., and Kutty, T. R. N., *A Basic Course in Crystallography*, Publishers: Universities Press, Year: **2001**.
2. Giacavazzo, C., *Fundamentals of Crystallography*. Publishers:Oxford University Press, Edition: Second, Year: **2002**.
3. Hammond, C., *Basics of Crystallography and Diffraction*, Publishers: Oxford University Press, Edition: Third, Year:**2009**
4. Stout G. H., and Jensen, L. H., *X-ray Structure determination: A practical guide*, Publishers: John Wiley & Sons, Edition: Second, Year: **1989**.

CHM 609: Organometallics (4)

Prerequisites (Desirable): *CHM 204, CHM 301, CHM 302*

Learning Objectives

To understand and apply the concepts of organometallic chemistry in various homogeneous and heterogeneous catalytic processes.

Course Contents

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 Books*:**

1. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*, 3rd Ed.; Wiley-Interscience: New York, **2001**.
2. Hartwig, J. F. *Organotransition Metal Chemistry From Bonding to Catalysis*, 1st Ed.; University Science Books: Sausalito, CA, **2010**.
3. 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**.
4. Spessard, G.O.; Miessler, G.L. *Organometallic Chemistry*. Prentice Hall: Upper Saddle River, NJ, **1996**.
5. Huheey, J.E.; Keiter, E.A.; Keiter, R.L. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Ed.; HarperCollins: New York, **1993**.
6. Jordan, R. B. *Reaction Mechanisms of Inorganic and Organometallic Systems;*2nd Ed.; Oxford University Press: Oxford, **1998**.
7. (a) Bochmann, M. *Organometallics 1;* Oxford University Press: New York, 1994. (b) Bochmann, M. *Organometallics 2;* Oxford University Press: New York, **1994**.
8. Elschenbroich, C.; Salzer, A. *Organometallics: A Concise Introduction*, 2nd Ed.; VCH: New York, **1992**.
9. Shriver, D. F.; Atkins, P. W. *Inorganic Chemistry*, 3rd Ed.; W. H. Freeman: New York, **1999**.
10. Attwood, J. D. *Inorganic and Organometallic Reaction Mechanisms*, 2nd Ed.; VCH Publishers Inc.: New York, **1997**.
11. Nugent, W. A.; Mayer, J. A. *Metal-Ligand Multiple Bonds*, 1st Ed.; Wiley-Interscience, **1987**.
12. Elschenbroich, C. *Organometallics, 3rd, Completely Revised and Extended Edition;*Wiley-VCH Verlag GbmH & Co. KGaA, Weinheim, Germany, **2006**.
13. Cotton, F. A.; Murillo, C. A.; Walton, R. A. *Multiple Bonds between Metal Atoms*, 3rd Ed.; Springer Science Inc. New York, **2005**.
14. Primary literature (journal articles).

CHM 612: Advanced Organic Chemistry – II (4)

Prerequisites (Desirable): *CHM 311, CHM 312*

Learning Objectives

This course discusses the philosophy of synthetic design for preparing complex chemical entities of natural and synthetic origin.

Course Contents

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 Books*:**

1. Clayden, J. et al., *Organic Chemistry*, 2^{nd} Ed., Oxford University Press, **2001**.
2. Wyatt, P. and Warren, S., *Organic Synthesis: Strategy and Control*, Wiley-Blackwell, **2007**.
3. Warren, S., *Organic Synthesis: The Disconnection Approach*, Wiley, **1983**.
4. Nicolaou, K. C. and, Sorensen, E., *Classics in Total Synthesis*, Wiley-VCH, **2008**.
5. Nicolaou, K. C. and Snyder, S. A., *Classics in Total Synthesis-II*, Wiley-VCH, **2003**.
6. Corey, E. J. and Cheng, X-M., *The Logic of Chemical Synthesis*, Wiley, **1995**.

CHM 613: Advanced Organic Chemistry – I (4)

Prerequisites (Desirable): 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 Books

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

CHM 614: Advanced Organic Chemistry – III (4)

Prerequisites (Desirable): CHM 312, CHM 313

Learning Objectives

This advanced course details the utility of organometallic complexes as catalysts for undertaking organic transformations. It also builds the concepts and principles involved in design of ligands and complexes for specialized purposes such as olefin metathesis.

Course Contents

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 Books

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

CHM 615: Frontiers in Organic Chemistry (4)

Prerequisites (Desirable): *CHM 311, CHM 312*

Learning Objectives

This course explores the most recent advances in Organic Chemistry as reported in the recent scientific literature.

Course Contents

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 Books

1. Research articles published in scientific journals.
2. Carriera, E. M. and Kvaerno, L., *Classics in Stereoselective synthesis*, Wiley-VCH, **2008**.
3. Hudlicky, T. and Reed, J. W., *The Way of Synthesis*, Wiley-VCH, **2007**.
4. Kurti, L. and Czako, B., *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier, **2005**.
5. Nicolaou, K. C. and Sorensen, E., *Classics in Total Synthesis*, Wiley-VCH, **2008**.
6. Nicolaou, K. C. and Snyder, S. A., *Classics in Total Synthesis-II*, Wiley-VCH, **2007**.

CHM 617: Chemical Biology (4)

Prerequisites (Desirable): *CHM 311, CHM 312, CHM 343*

Learning Objectives

This course covers the advanced topics related to Chemistry involved and utilized in altering biological processes. Synthesis and utilization of bioconjugates and design of functional mimics of biomolecules is covered in this course.

Course Contents

Introduction: What is Chemical Biology? Basics of Biology: Lipids, DNA, Protein, Sugars.

Nucleic acids: Structure and function of DNA and RNA and their modulation. Molecular recognition of DNA, RNAi, DNA/RNA Nanotechnology.

Peptides and proteins: Structure and function of proteins and their modulation, Protein folding and misfolding. Protein-protein interactions.

Bioorthogonal Ligation techniques: Functional group specific ligation techniques, Staudinger Ligation, Native Chemical Ligation, Intein-mediated synthesis, Site selective protein modification.

Lipids: Natural and synthetic membranes and their applications.

Microscopy and Spectroscopy in Chemical Biology: Scope and application of various microscopic and spectroscopic tools to investigate biomolecules.

Synthetic functional mimetics of biomolecules.

Suggested Books

1. Waldmann, H., *Chemical Biology: Learning Through Case Studies*, Wiley-VCH, **2009**.
2. Dobson, C. M., Gerrard, J. A. and Pratt, A. J., *Foundations of Chemical Biology*, Oxford Univ. Press; **2002**.
3. Miller, A. D. and Tanner, J., *Essentials Of Chemical Biology: Structure and Dynamics of Biological Macromolecules*, Wiley, **2002**.
4. Waldman, H. and Janning, P., *Chemical Biology: A Practical Course*, Wiley-VCH, **2004**.
5. Hermanson, G. T., *Bioconjugate Techniques*, Academic Press, **2008**.
6. Lackowicz, J. R., *Principles of Fluorescence Spectroscopy*, 3rd Ed., Springer, **2006**.
7. Journal Articles

CHM 624: Molecular Simulations (4)

Prerequisites (Desirable): *CHM222, CHM322, CHM421*

Learning Objectives

The aim of this course is to provide a solid background necessary to design and carry out molecular simulations. The course will cover a wide range of techniques for simulating physical and chemical processes in the condensed phase. The methods for molecular dynamics and Monte Carlo simulations will be described and will involve applying these methods to calculate various structural, thermodynamic, and dynamic properties of matter. Subsequently techniques for calculating free energies and phase equilibria, advanced sampling strategies, and coarse-graining will be discussed. A major emphasis of the course is on getting hands-on experience on computer simulations.

Course Contents

Introduction: 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.

Basic methods: Description of semi-empirical **f**orce-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 Books*:**

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

CHM 625: Biophysical Chemistry (4)

Prerequisites (Desirable): *CHM222, CHM 321, CHM322, CHM421/CHM621*

Learning Objectives

This is an elective course for Ph.D. students in the Chemistry department. It is also a departmental elective for 4th and upper year Chemistry majors as well as an open elective for 4th and upper year BS-MS students from other departments meeting the pre-requisites below. 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 Books*:**

1. Cantor, C. R., and Schimmel, P., *Biophysical Chemistry (parts I, II and III)*, W. H. Freeman, **1980**.
2. Jackson, M. B., *Molecular and Cellular Biophysics*, Cambridge, **2006**.
3. Serdyuk, I. N., Zaccai, N. R.,and Zaccai, J.,*Methods in Molecular Biophysics: Structure, Dynamics, Function*, Cambridge, **2007**.
4. Daune, M., *Molecular Biophysics: Structures in Motion*, Oxford, **1999**.
5. Lakowicz, J. R., *Principles of Fluorescence Spectroscopy*, Plenum Press, **2003**.

CHM 627: Fundamentals of NMR Spectroscopy: Principles and Applications (4)

Prerequisites (Desirable): *CHM 322, CHM 402/416, CHM 422/622*

Learning Objectives

The theoretical basis of NMR experiments that are applied to study molecular structure and dynamics will be described. Principles of Fourier transform NMR will be discussed with emphasis on instrumentation, data acquisition, processing and analysis of multidimensional NMR experiments. Routine experiments would be understood from the fundamentals on how such spectra are acquired, in addition to their practical aspects/applications.

Course Contents

Classical NMR spectroscopy: Nuclear magnetism, the Bloch equations, one-pulse experiment, line-width and chemical shift, scalar coupling.

Theoretical description of NMR spectroscopy: Brief introduction to quantum mechanics, Liouville-von Neumann equation, rotating frame transformation, density matrix representations, pulses and rotations, quantum mechanical description of NMR spectroscopy, extension to multiple spin systems, the one pulse experiment, concept of coherence, product operator formalism and its applications to single/multiple quantum coherence experiments.

Practical aspects of NMR spectroscopy: NMR instrumentation, experimental set up, data acquisition, data processing (introduction to Fourier transformation), pulse, z-axis gradients and spin-decoupling techniques, extension to methodology to two- and multidimensional experiments.

Chemical applications: Basic 1D ^{1}H NMR experiments (including solvent suppression), nuclear Overhauser effect spectroscopy, 2D NOESY and ROESY, correlation spectroscopy (COSY and its variants), total correlation spectroscopy (TOCSY), J-resolved spectroscopy, diffusion ordered spectroscopy (DOSY), concept of polarization and coherence transfer (INEPT), heteronuclear correlation experiments (HETCOR, HSQC, HMQC, HMBC).

Biological applications: 2D [^{15}N, ^{1}H] and [^{13}C, ^{1}H] HSQC, transverse relaxation optimized spectroscopy (TROSY), common 3D NMR experiments (HNCO, HNCαCβ, CβCα(CO)NH, HβHα(CO)NH, (H)CCH-COSY, (H)CCH-TOCSY, HSQC-NOESY, NOESY-HSQC), rapid data acquisition techniques, residual dipolar couplings, conventional and recent advances in structure determination of proteins and nucleic acids.

Relaxation and dynamic processes: Steady-state and transient NOE, Solomon's equations and its applications, chemical and conformational exchange, Bloch equations, the relaxation master equation, spectral density functions, relaxation mechanisms.

Suggested Books

1. Cavanagh, J. *et al.*, *Protein NMR Spectroscopy, Principles and Practice*. 2nd Ed., Elsevier, **2007**.
2. Levitt, M.H., *Spin Dynamics: Basics of Nuclear Magnetic Resonance*, 2nd Ed. Wiley, 2008.
3. Ernst, R.R., *et al.*, *Principles of Nuclear Magnetic Resonance in One and Two Dimensions*, Clarendon Press Oxford, **1987**.
4. Rule, G.S. and Hitchens, T.K., *Fundamentals of Protein NMR Spectroscopy*, Springer Netherlands, **2006**.

CHM 628: Electrochemistry: Fundamentals and Applications (4)

Prerequisites (Desirable): *CHM 321*

Learning Objectives

The prime objective of this course is to understand fundamentals of basic electrochemistry. Second part of the course highlights utilization of fundamental knowledge towards application of different laboratory electrochemical techniques and its practical implication in renewable energy research.

Course Contents

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 Books

1. Bard, A.J. and Faulkner, L.R., *Electrochemical Methods: Fundamentals and Applications*, 2nd Ed, John Wiley & Sons, **2001**.
2. Bockris, J.O'M, Reddy, A.K.N, *Modern Electrochemistry Ionics: Volume 1*, 2nd Ed., Plenum Press, **1998**.
3. Recent Research Publications.

CHM 629: Advanced Molecular Spectroscopy (4)

Prerequisites (Desirable): *CHM 322/642, CHM 422/622*

Learning Objectives

The objective here is to have a thorough understanding of both theoretical and practical aspects of molecular spectroscopy. The radiative processes, namely fluorescence and phosporescence and their theory will be discussed, special emphasis will be given to associated instrumentations. Finally, the nuances of single molecule spectroscopy and time-correlated single photon counting and its applications will be dealt with.

Course Contents

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 Books*:**

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

CHM 630: Advanced Statistical Mechanics (4)

Prerequisites (Desirable): *CHM322/CHM642, CHM421*

Learning Objectives

This course builds on the concepts introduced in CHM 421 and this graduate level course intends to introduce some advanced topics in the field of statistical mechanics and their application to various physical systems. The main objective of this course is to introduce simple models of these systems and develop approaches for solving them. It is aimed primarily at students engaged in interdisciplinary research activities across multiple disciplines.

Course Contents

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 expansion 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 Books*:**

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

CHM 631: Electronic Structure (4)

Prerequisites (Desirable): *CHM 633*

Learning Objectives

This course is aimed at students interested in learning and working with density-functional theory (DFT) and follows courses on basic quantum chemistry. Both formal as well as practical aspects of DFT will be introduced in the course. The course will also feature hands-on sessions to learn popular DFT codes.

Course Contents

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 (DFT) – 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 Books

1. W. Koch and M. Holthausen, *A chemist's guide to density-functional theory*, John Wiley & Sons, **2001**.
2. A. Szabo and N. S. Ostlund., *Modern Quantum Chemistry*, Dover Publications, **1989**.
3. R. Martin, *Electronic Structure.* R.G. Parr and W. Yang, *Density-functional theory of Atoms and Molecules*, Oxford Science Publications, **1995**.

CHM 632: Physical Chemistry of Polymers (4)

Prerequisites (Desirable): *CHM 222, CHM 321, CHM 324, CHM 421*

Learning Objectives

This graduate-level course is an introduction to the fundamental physical chemistry and physics of polymeric systems. The kinetics of polymerizations, structure, and properties of polymer solutions, gels, rubber networks and crystalline state of polymers are the main themes of discussion. The course will also introduce the application of polymers in organic optoelectronics aiming to develop an understanding of structure-property correlations.

Course Contents

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 Books

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

CHM 633: Advanced Quantum Chemistry (4)

Prerequisites (Desirable): *CHM 322/642*

Learning Objectives

This is an elective course for Ph.D. students in the Chemistry department. It is also a departmental elective for 4^{th} and upper year Chemistry majors as well as an open elective for 4^{th} and upper year BS-MS students from other departments meeting the pre-requisites below. The course is a first introduction to electronic structure theory and aims at providing both qualitative and quantitative understanding of chemical binding. The course covers topics relevant for understanding practical quantum chemistry such as orbital and spin angular momenta and their addition, many-electron wavefunctions, slater determinants, Hartree-Fock theory and the SCF method, post-HF theories and a brief introduction to density-functional theory.

Course Contents

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 H_2^+ 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 Books

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

CHM 637: Chemistry and Physics of Materials (4)

Prerequisites (Desirable): *CHM 222, CHM 322/642*

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, absorption 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 Books*:**

1. Gersten, J.I. and Smith, F.W., *The Physics and Chemistry of Materials*, John Wiley & Sons, **2001**.
2. DiVentra, M. *et al.*, *Introduction to Nano-science and Nano-technology*, John Wiley & Sons, **2010.**
3. Grosso, G. and Parravicini, G., *Solid State Physics*, Elsevier, **2013**.

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

Prerequisites (Desirable): *CHM 322/642*

Learning Objectives

This course aims to introduce the topic of non-adiabatic dynamics in molecular and condensed phase systems. A formal development of the topic along with suitable examples will be presented to prepare graduate students for research on non-adiabatic effects in chemical, physical and biological systems.

Course Contents

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 Books*:**

1. Baer, .M and Ng, C-Y, *State-Selected and State-to-State Ion-Molecule Reaction Dynamics. Ser. Advances of Chemical Physics*, Vol. 82, Part 2, John Wiley & Sons, **1992**.
2. Baer, .M and Billing, G.D., *The Role of Degenerate States in Chemistry*, Ser. Advances of Chemical Physics, Vol. 124; John Wiley & Sons, **2002**.
3. Domcke, W., *et al.*, *Conical Intersections*, Advances Series in Physical Chemistry Vol. 15, World Scientific, **2004**.
4. Farad. *Discussions, Non-Adiabatic Effects in Chemical Dynamics,* Vol. 127, Royal Society of Chemistry, **2004**.
5. Baer, .M, *Beyond Born-Oppenheimer: Electronic Nonadiabatic Coupling Terms and Conical Intersections*, Wiley Interscience, **2006**.
6. Schatz, G.C. and Ratner, M. A., *Quantum Mechanics in Chemistry*, Prentice-Hall, **1993**.
7. Jackson, J.D., *Classical Electrodynamics*, 2nd Ed., John Wiley & Sons, **1975**.
8. Zhang, J. Z. H., *Theory and Application of Quantum Molecular Dynamics*, World Scientific, **1999**.