Chemistry curriculum

2019

CHEMISTRY UNBOUND: An outcome of continued, collective and collaborative effort with a vision to develop an innovative, responsive, inclusive, flexible and dynamic curriculum in tune with the global educational needs for the 21st century and beyond

Department of Chemistry

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Contents

Vision & Mission

Discover

Create

Understand

Inspire

Educate

Lead

Collaborate

Department of Chemistry

Department of Chemistry, Pondicherry University, since its inception is a leader and trend setter in developing and implementing a relevant model curriculum which has been adapted by several premier institutes in India. Chemistry curriculum 2019, called *Chemistry Unbound*, is an outcome of our continued, collective and collaborative effort with a vision to develop an innovative, responsive, inclusive, flexible and dynamic curriculum in tune with the global educational needs for the 21st century and the National education policy 2019. Our curricular structure, courses, pedagogy and assessment has truly catered to the development of diversified, integrated, interdisciplinary knowledge and skills as well as inculcation of the values to survive in the highly competitive knowledge and skilled society.

Vision and Mission

To boldly explore and advance new chemical frontiers in the life sciences, physical sciences, medicine, energy, materials, and environmental sciences through visionary research, innovation, collaboration, and scholarship

Discover, Create and Understand

Design and model molecules that modulate biological processes

Create materials for energy storage, reaction enhancements, and applied materials

Understand the contribution of geometric and electronic structure to function

Inspire and Educate

Inspire a knowledge platform that supports an inventive culture

Educate future leaders about how chemistry underlies living systems and physical processes

Lead and Collaborate

Lead in fostering solutions to problems of global significance by collaborating across many disciplines both within and external to Pondicherry University

To achieve these aims the Chemistry at Pondicherry University must continue to evolve the cutting-edge facilities, world-leading faculty, and top-quality student body that will make transformative science possible.

Vision

Chemists are driving a molecular revolution of unprecedented magnitude and impact, that will transform whole of science and the world as we know it. Chemistry—the quintessential molecular science—is enabling us to "see and explore" with atomistic resolution, these previously unobservable scientific frontiers.

With this new knowledge, chemists have created remarkable new molecules, materials, tools and theories for the benefit of science and society. We can now make, modify, simulate and interrogate most molecules that have ever existed. Equally importantly, we can design, make and study fascinating new ones.

Chemistry at Pondicherry University is a leader of the molecular revolution, addressing the most challenging and important questions in the physical and life sciences of the 21st century. By leveraging its multi-disciplinary vision, its culture of synergistic collaboration and translational science, and its excellence in the physical, biological and engineering sciences, Chemistry at Pondicherry University is opening new fields and frontiers and fundamentally new and innovative ways to address the increasingly complex scientific, health, energy and environmental problems of our time.

Mission

Discover, Create and Understand

Through independent research and synergistic collaborations with scientists and entrepreneurs around the world, the department continues to build on its distinguished history of major advances in chemical science and computation, creating innovations that open new research opportunities multiple domains of sciences.

Inspire and Educate

Through spirited mentoring of future researchers, innovative instruction of students within chemistry and across majors, and creative approaches to scientific communication, visualization and computation, the department trains and informs tomorrow’s leading scientists, professionals and policymakers, and fosters new knowledge of the chemistries underlying living systems and physical processes.

- Inspiring and educating undergraduate students in chemistry and molecular-driven sciences in the core concepts of chemistry and scientific methods.

- Advancing a knowledge platform that supports an invent-and-design culture in graduate and undergraduate chemistry education, and that empowers students to address and solve challenges of global significance

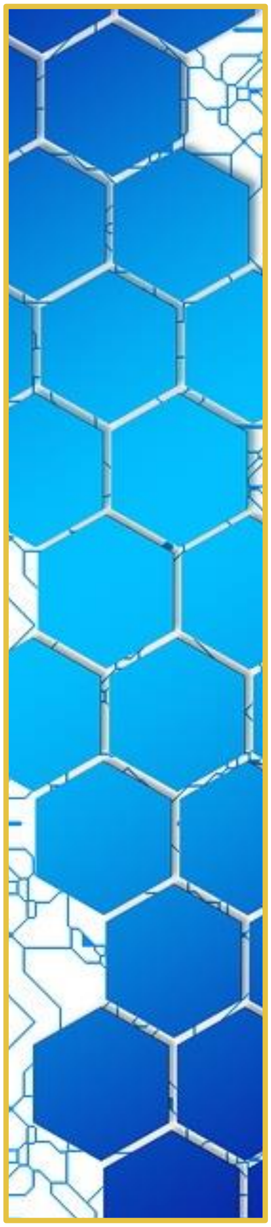
• Reaching out to our future thought leaders—students of all backgrounds from college to doctoral candidates—to share the power of chemistry to create new knowledge directed at the major unmet needs of our time

• Supporting and advancing worldwide community of chemistry scholars

• Informing the public about the excitement of science, its impact on everyday life, and the crucial role it plays in human health, energy and environmental stewardship

Lead and Collaborate

The Chemistry Department is blazing a path of excellence that will define the future of scholarship in the chemical sciences by supporting a creative environment that fosters discovery, learning and collaboration, and by drawing the best faculty and students to the university.



Ph.D. Chemistry

Lead in fostering solutions to problems of global significance by collaborating across many disciplines.

Ph.D. Chemistry

Department of chemistry, Pondicherry University, since its inception is actively involved in research in the frontier areas of chemistry. All faculty members, Inspire Fellows, Young Scientists, Post-Doctorate fellows have generated lot of interests among prospective research students. Department of chemistry actively generate resources from various government, private funding agencies in addition to university resources.

Pondicherry University and Department of Chemistry houses numerous states of the art instrumentations.

Students shall register CHEM670 as a mandatory theory paper (Paper I) during their first year of their research program. Students shall register one additional paper (Paper II) in consultation with their research guide/mentor. This curriculum also gives contents of various topics. Research supervisors/mentors may recommend one or more courses from this list. Alternatively, research supervisor/mentor may recommend any other course as per their requirements. In addition, research supervisors/mentors shall make necessary arrangements to place the course contents of both Paper-I and Paper-II in the respective doctoral committee for approval.

Students shall write three hours written examination at a mutually convenient date and time. The evaluated grades/marks shall be placed in the Doctoral Committee and uploaded in the university SAMS portal

CHEM670 Research Methodology

Credit: 6

Pre-requisite: M.Sc. Chemistry or equivalent

Course Content:

Unit I The Methodology

Literature survey - Journals, books and databases – Search Engines for chemistry research – Following the Bibliographic trail - Managing References.

Research processes - scientific research, formation of the topic, hypothesis, conceptual definitions, operational definition, gathering of data, analysis of data, revising of hypothesis, Managing chemical Data using Software - Conclusion.

Errors in chemical analysis, classification of errors, determination of accuracy of methods – calibration of Data.

Effective Presentation of Literature and research output in Orals and Posters – Processing of Images & animated content in Power-point presentations – Methodology of citing references.

Publication of Research Papers – Articles, Communications, overviews and reviews – Identifying Avoiding Plagiarism – Principles for Clear writing – Effective ways for Planning, Drafting and Revising Manuscripts – Using Templates & reference Managers.

Unit II Lab Safety

Principles, Ethics and Practices

Emergency response and containment – Fire emergencies in organic labs – Chemical spills - First Aid

Understanding and recognizing lab hazards –The language of safety – signs, symbols and Labels – MSDS and GHS

Toxic substances and biological agents – Acute and chronic toxicity – carcinogens – Bio-accumulation

Physical Hazards-– Gas cylinders and cryogenics – High/low pressure hazards – Electric& Radiation Hazards

Chemical Hazards - Flammables, Corrosives and Explosives – Incompatibles - Runaway reactions

Managing Hazards – Eye, Face and skin Protection –Protective clothing, Gear and Respiratory

Managing Chemicals – Handling Waste – Storing inflammables and corrosives – Inventory and Self-Inspection

Unit III Handling of Instruments

Disciplinary Practices in handling various equipment – Maintenance – Logging & Trouble-shooting

Preparation of samples and Basic skills for handing IR/UV – NMR – XRD – EPR – CHN Analyser – GC - CV – Glove box

Using Computational Facility- Available Copyrighted Chemical Software & Systems – Introduction to Gaussian 09 and other modelling software - Maintenance of Computers – Linux and Windows Basics – Hardware basics and Troubleshooting.

References

Hill, R. H. Jr. &Finster, D. C. “Laboratory Safety for Chemistry Students”, 2ndEdn., John Wiley & Sons, 2016.

Booth, W. C. Colomb,G. G.; Williams, J. M. ; Bizup, J. ; FitzGeraldW. T., “The Craft of Research”, 4thEdn, Univ. Chicago Press, 2016.

Alley, M., “The Craft of Scientific Presentations”, 3nd Edn., Springer, 2013.

Hibbert D. B; Gooding J. J., “Data Analysis for chemistry”, Oxford, 2016.

CHEM671: Fundamentals of Molecular Structure

Credits: 6

Pre-requisite: M.Sc. Chemistry or equivalent

Unit I Symmetry Groups

Group Theory Basics – Symmetry Elements, Operations & relationships – Schoenflies Point Groups - Matrix representation and its Character – Classes of symmetry operations - The Great Orthogonality Theorem (without proof) – Construction and Usage of Character tables – Reducible and Irreducible representations – Direct Products – Projection operators.

Unit II Stereochemistry: The Chemistry of Shapes

Polyhedral Types – Vertex, Edge and Face Transitivity – Configuration and Conformation – Tetrahedron & Stereoisomers – Conformations around different σ-bonds - Geometries of Mono/polycyclic systems – Conformational entropy - higher (5-12) coordination – Distortions – Chelation isomers – Substituent Permutations – Vertex, axial, planar, helical and pro-chirality – Multiple Chiral Centres - Optical activity – Nomenclature.

Unit III Electronic Spectra

Nature of electromagnetic radiation – Interaction with matter – Electronic energy levels and CI - SALC – Absorption and Emission – Transition moments and probability – Selection rules – Intensities - Broadening – Vibronic transitions –

Frank-Condon Principle – Vibrational progressions and excited state geometry – Radiative and Non-radiative decay - XPS & Auger electron spectra.

UNIT IV Rotational and Vibrational Spectra

Pure Vibrational and Rotational spectra - Spectra of Di and Polyatomics - Normal Modes symmetry - Selection rules – Fermi Resonance – Anharmonicity and Isotope effect – Determination of Bond-lengths and Bond strengths – Vibrational Localization of Functional groups – Polarizability and Raman effect - Rotational and Vib-Rotational Raman spectra - Exclusion Rule.

UNIT IV Solids and Diffraction methods

Bravais Lattices – FCC and HCP – Unit cells types – Reciprocal lattice – Brillouin zone – Miller Indices – Classification of Crystal systems & Bravais lattices – Crystallographic Point and Space Groups – 2D-Lattices – XRD and Bragg’s law – Lau, Debye-Scherrer, Bragg methods – Systematic Absences – Structure and Form Factors – Phase problem – Absolute configuration - Electron Diffraction and LEED.

Recommended Books:

F. A. Cotton, Chemical applications of Group Theory (3rd Edition), John-Wiley & Sons, 2003.

E. L. Eliel & S. H. Wilen, Stereochemistry of Organic Compounds, John-Wiley & Sons, 1994.

P. W Atkins & J. de Paula: Physical Chemistry (10th Edition), Freeman & Co, 2014.

N. W. Ashcroft & N. D. Mermin, Solid State Physics, Harcourt Inc., 1976.

CHEM672: Chemistry Principles in Reaction Energetics

Credits: 6

Pre-requisite: M.Sc. Chemistry or equivalent

Unit I Equilibrium Thermodynamics

Review of classical thermodynamics – Temperature, Energy, Entropy - Nernst Theorem – Gibbs and Helmholtz Free energy – Chemical Potential – Partial molar properties and their significance – Fugacity and its Determination – Non ideal systems – Activity, Activity coefficients – Debye-Huckel theory of electrolytes – ionic strength – Phase rule for three component systems – Second order Phase transitions - The Ehrenfest classification.

Unit II Chemical equilibrium

Reaction Gibbs energy - Exergonic and endergonic reactions - Equilibrium constants and their inter-relations – Molecular Interpretation – Response to Pressure and Temperature – Electrochemical cells - Half-reactions and electrodes – Types of cells and potentials - The Nernst equation – Determination of reaction entropies and enthalpies - Electrode potentials Measurement and applications – Electrochemical series.

Unit III Statistical Thermodynamics

The Boltzmann distribution – Molecular Partition functions and thermodynamic properties – Molecular energies - translational, rotational, vibrational, electronic contributions – Ensembles – Averaging Postulates – Mean energy and its variation – Entropy, internal energy and partition functions – Heat Capacity-Residual entropies – Equilibrium constants - Fermi-Dirac statistics and metals - Bose-Eienstein statistics and helium.

Unit IV Non-Equilibrium Thermodynamics

Criteria for Non-Equilibrium States – Entropy Production and flow – flux-force relationship – non-equilibrium Stationary states – Phenomenological equations – microscopic reversibitily – Onsager's reciprocity relations – Electrokinetic phenomena – Diffusion – Electric Conduction - Electrochemical Potential – Steady State Entropy – Coupled Reactions.

Unit V Thermochemistry

Enthalpies of Physical and chemical Changes – Hess Law – Enthalpy of combustion and Formation - Reaction enthalpy from enthalpy of formation – Temperature Dependence – DSC & DTA - Concepts of Strain and Stability in molecules – Bond energy - Bond Dissociation energy Bond strength – Isodesmic equations – Benson Group Increment Theory – Atomic and ionic Radius – Lattice energies – Heats of ligation and Stability constants for metal complexes.

Recommended Books:

P. W Atkins & J. D. Paula, Physical chemistry, 10th Edition, W. H. Freeman & co.

T. Engel, P. Reid, W. Hehre, Physical chemistry, 3rd Edition,

D. A. McQuarrie & J. D. Simon, Physical Chemistry, 1st Edition, University Science.

E.V.Anslyn & D. A. Dougherty, Modern Physical Organic Chemistry, University Science.

CHEM673: Electronic Structure of Elements and Molecules

Credits: 6

Pre-requisite: M.Sc. Chemistry or equivalent

Course Content:

Unit I Solving Schrodinger's One Electron Atom

The Schrödinger equation – Atomic units – Transformations Relative coordinates - Schrodinger equation in spherical polar coordinates – Separation of variables – Spherical Harmonics – Legendre Equation and its solutions – Interdependency of l and m – The Radial equation and its simplification – Asymptotic solution for ρ equation – interdependency of l and n – Laguerre and associated Laguerre polynomials.

Unit II Nature of Hydrogenic Wave-functions

Energies and Degeneracies – Justification for Bohr's Energy and Rydberg's formula - Virial Theorem - Angular Momentum – Expressions for Atomic Orbitals – Radial Plots – Probability and Radial Distribution plots – Average and Most probable Distances – Impact of Nuclear Charge variation – Polar plots – Shapes of Atomic orbitals – Planar, Radial Nodes and Orthogonality.

Unit III Approximations for many-electron Schrodinger equation

Atomic Hamiltonian - Independent Electron Model - Theory of Perturbation - Non-degenerate Perturbation theory - I & II Order Corrections –– Perturbation

Treatment of He – Degenerate Perturbation – Theory of Variation – Linear and non-linear Variation – Matrix formulation of Linear Variation - Secular Determinant - Variational treatment of He – Effective nuclear charge.

Unit IV Atomic Structure of many electron atoms

Quantum Particles Indistinguishablity – Electron Spin and its interpretations – Pauli's Antisymmetry principle – Excited states of Helium - Nature of Exchange – Slater Determinants - Slater Type Orbitals – Aufbau principle – Deconstruction of Periodic table – Electron Angular momentum and Spin-Orbit Coupling – Evaluations for Total Angular momentum – Term Symbols – Hund's Rules and its limitations.

Unit V Electronic Structure of Molecules

Bonn-Oppenheimer Approximation – Electronic structure of H2+ - Ground and Excited states of H2 – LCAO-MO Theory - VB Theory – Nature of Exchange - HF-SCF Theory – Definition of Chemical bond – Correlation - Configuration interaction - Electronic structure of Homo and Hetero Diatomics of Second Row – Bonds & Lonepairs vs MOs – Bond order - sp Mixing and Avoided Crossing - MO Configuration – Electronic States and Term Symbols.

Recommended Books:

I. N. Levine, Quantum Chemistry, 7th edition, Prentice Hall.

D. J. Griffiths, Introduction to Quantum mechanics, 2nd Edition.

J. P. Lowe & K. A. Peterson, Quantum Chemistry, 2nd edition, Elsevier Academic.

P. W Atkins & R. S. Friedman: Molecular Quantum Mechanics, 4th Edition, Oxford.

D. A. McQuarrie, Quantum Chemistry, Ist & IInd Editions, Pearson.

CHEM674: Principles of Chemical Bonding

Credits: 6

Pre-requisite: M.Sc. Chemistry or equivalent

Course Content:

Unit I Localized Octet Bonding involving s & p Elements

Review of Classical Bonding ideas – Molecular geometry – Hybridization theory – isovalent hybridization – Bent's rule - VSEPR Theory – FMO theory –- Fundamentals of FMO interaction – Avoided crossing – Jahn-Teller distortions - FMOs of AHn (n=1-4) systems – FMOs A2Hn and ABHN systems – Electronegativity and its perturbation - Bonding in Small rings .

Unit II Delocalized Bonding: Huckel & its Extensions

The simple Huckel method – Assumptions – Determinant, Energies and Wave functions – Extended Huckel & Overlap - Population Analysis – Interaction and Walsh diagrams – Conjugation and Aromaticity – Heteroaromaticity – FMOs of Functional groups – Substitutent effects - Hyperconjugation and Anomeric effect – 3D Conjugation - Inorganic Rings.

Unit III Nature of Bonding in compounds Transition metals

Review of VB, CFT and LFT – Octahedral, square planar and Tetrahedral complexes – Limitations - MO theory – Electron counting – Bond Strengths and Lability – HSAB theory -Chelate effect - EAN rule and Organometallics – Tm-Carbon interactions - Complexes of CO, NO, N2 and O2 - Distortions - $p\pi$-$d\pi$

bonding – Tm-Tm bonding - Square-planar vs Tetrahedral preferences – TBP vs Square Pyramidal - FMOs of MLn fragments – Isolobal analogy.

Unit IV Periodicity and Diagonal relations

The first and Second Row anomalies – Primogenic repulsion – Impact of Radial nodes – π-bonding in heavier main group – Trans bending – Inert-pair effect – spin orbit coupling and Relativistic effects – Diagonal Relationships and its Variation - Extent of d orbitals influence in non-metals – Heavier s block - Periodic anomalies of transition metals.

Unit V Bonding in Electron Rich/Deficient & Hyper/Hypo Valent compounds

Diborane – 3c-2e formalism and its drawbacks – Polyhedral boranes – Wade's rule and its extensions – Extension of aromaticity to polyhedra – Heavier analogs – Tm clusters – Mingos rules – Hypervalent compounds – Bonding in Oh, D3h, D4h, C4h symmetric AXn systmes of heavier p block elements – Multiple Bonding in molecular [AOn] [TmOn] species.

Unit VI Bonding in Solids

Orbitals in periodic potential - Bloch functions and k-space - 1D-Chains & 2D sheets – Energy Bands – Direction and width – Avoided crossings – Folding of bands – Distortions – Density of States and its Projections – Electronic structure of solids – Fermi Energy – Semiconductors, metals and insulators – Band-gap engineering - Population analysis – surface Bonding.

Recommended Books:

TA Albert, JK Burdett, & MH Whangbo, Orbital Interactions in chemistry, 2nd edition, Wiley.

JP Lowe & KA Peterson, Quantum Chemistry, 3rd Edition, Elsevier.

JE Huhee, EA Keiter & RL KEITER Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edition, Hypercollins.

R Hoffmann, Solids and Curfaces: A Chemists view of Bonding in extended structures, 1st Edition, Wiley.

CHEM681: Concepts in Chemical Kinetics

Credits: 6

Pre-requisite: M.Sc. Chemistry or equivalent

Course Content

Unit I Free Energy Relationships

Review of Rate law, Rate constants and order - Free energy of activation - Linear Gibbs energy relations – Edward's Equation and alpha effect - Theories of Acids and bases - Equilibrium constant - kinetic effects - Thermodynamic and kinetic control of reactions. Hammond postulate, Curtin-Hammett principle - Hammett equation and its Applications.

Unit II Reaction Dynamics

Collision theory – Lindemann-Hinshelwood and RRKM model – Diffusion control – Molecular Beams & collisions - Transition state theory – Eyring equation – Barrier less reactions - Activated complex – Arrhenius equation - kinetic isotope effect – Kramer's theory -Statistical approach to transition states – PES of Excited states - Conical Intersections & avoided crossings – Spin-orbit coupling – branching and seam spaces.

Unit III Photo & Fast Reactions

Photophysics of Unimolecular processes – Delayed fluorescence – Kinetics of bimolecular processes – Collision quenching – Stern-Volmer relations – Concentration dependence of quenching – Excimers – electron transfer in

Excited state – Exciplex, Twisted intramolecular charge transfer processes - proton couple electron transfer processes – Features of fast reactions – study by flow method – relaxation methods – Flash photolysis.

Unit IV Kinetics of Surfaces and Catalysis

Solid surfaces and its growth – Physisorption and Chemisorption – Adsorption and Desorption – Adsorption isotherms – Rate and extent of adsorption and desorption – Experimental assessment – molecular picture of adsorption and mobility – Catalysis – General Principles – Heterogenous and Homogenous catalysis – Catalysts and its types – Mechanisms – Catalytic cycles – enzyme kinetics.

Unit V Kinetics of Electron transfer and Electrodes

Electron transfer in homogenous systems - rate law and rate constant – tunnelling –reorganization – Markus-Hush theory - Electrical Double layer – Electrode solution interface - Butler–Volmer equation – Tafel Plots – Voltammetry – Cyclic voltammetry and its applications – Electrolysis – working Principles of Galvanic cells – Nature of Electrochemical reactions – Mechanistic elucidation of electrode reactions.

Recommended Books:

P. W Atkins & J. D. Paula, Physical chemistry, 10th Edition, W. H. Freeman & co.

T. Engel, P. Reid, W. Hehre, Physical chemistry, 3rd Edition,

D. A. McQuarrie & J. D. Simon, Physical Chemistry, Ist Editions, University Science.

E.V.Anslyn & D. A. Dougherty, Modern Physical Organic Chemistry, University Science.

CHEM682: Reaction Mechanisms

Credits: 6

Pre-requisite: M.Sc. Chemistry or equivalent

Course Content

Unit I Reaction Mechanisms Fundamentals

Frontier Orbitals - Transition state Theory and its limitations – Topology of Transition states – Deciphering reaction mechanisms – Rate determining step and its identification – Molecularity – Perturbation theory of Reactivity - HSAB theory - Reactive Intermediates – Electronic Factors affecting their Relative Stability and Reactivity of Intermediates – Rearrangements – Neighbouring group participation – Steric hindrance and enhancements.

Unit II Frontier ‘sp’ orbitals with Linear Transition state

Nucleophiles, Electrophiles and Radicals – Nature of FMOs – Philosophy of Arrow Pushing - Unimolecular and bimolecular processes - Substitution in Saturated and Unsaturated systems – β and other Eliminations – Elimination vs substitution – Addition across Homo and Hetero nuclear multiple bonds – Electrophilic (Ar) and nucleophilic (RCOOR) Addition-Eliminations – Ring Closure Rules - Regio, Stereo and conformational preferences.

Unit III Frontier ‘sp’ orbitals with non-linear (Pericyclic) Transition state

Woodward-Hoffmann rules – Electrocyclic reactions – Con & Dis rotatory process - Cycloadditions - Diels-Alder and its Hetero, Retro & Asymmetric variants – Normal & Inverse e n demand - Sigmatropic reactions – Supra & Antra facial Shifts – NIH shift - Ene, Cheletropic and Dyatropic reactions – Site, Stereo, Regio & Peri selectivity – Concerted vs non-concerted pathways – Solvent effects – Arrow-pushing and its limitations- coarctate reactions.

Unit IV Mechanisms involving Frontier 'd' Orbitals

Ligand Exchange - Inert and labile complexes - – Association, dissociation and interchange – Aquation and SN1CB mechanism - Substitution in Square planar complexes – Trans effect, trans effect series – Steric effects - Octahedral complexes – Activation - Encounter complex - Cis effect – Ligand rearrangement and twisting – Redox reactions – inner sphere mechanism – Effect of Ligand Bridges – Outer Sphere mechanism – Intervalence electron transfer.

Unit V Organometallic reactions & Catalysis

Substitution in organometallic systems - Oxidative addition and Reductive elimination – Ionic and Radical mechanisms – Coupling and Fragmentation – CO and Alkene insertions & stereochemistry – Migratory insertion – carbo, hydro and trans metalation – β, α and other H eliminations – Template reactions – Homogenous Catalysis of π-bonds – Inert bond Activation – M-L Multiple bonding – Fischer/Schrock Carbenes – Reactivity of M-M bonds.

Unit VI Miscellaneous Reactions

Mechanistic Photochemistry – Conical intersections - Diabatic, adiabatic and hot reactions - Kinetic factors for quantum yields –Chemiluminescence - Energy and Electron transfer – Electrode Reaction kinetics – Reversal of Pericyclic rules – Electro-catalysis – Proton coupled Electron transfer – Reversal of Pericyclic rules – Electro-synthesis – Biochemical mechanisms - Structure and reactions of important cofactors – Enzymes, Coenzymes and Inhibitors.

Recommended Books:

I. Fleming, Molecular Orbitals and Organic Chemical Reactions, John-Wiley & Sons, 2009.

J. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley, 2014.

CHEM683: Molecular Spectroscopy

Credits: 6

Pre-requisite: M.Sc. Chemistry or equivalent

Course Content

Unit I Ionization spectra

Mass spectrometry - Basic principles, techniques of ion production and ion and daughter ions, molecular ion and isotope abundance, nitrogen rule, energetics of fragmentation - metastable ions, common fragmentation pathways – fragmentation pattern of common chemical classes – Ion-cyclotron Resonance – FTICR/MS – SIMS – LEED, AES and HREELS – STM and AFM – EXAFS and XANES.

Unit II UV-Visible Molecular Absorption Spectroscopy

Beer-Lambert Law – Electronic transitions (185-800nm) – Solvent effect – Saturated and unsaturated organic carbonyl compounds – Dienes & Conjugated Polyenes – Fieser-Woodward rules – Aromatic and heterocyclic compounds - Ground states of transition metal complexes – Correlation, Orgel and Tanabe-Sugano diagrams – Calculations of DQ, B and β parameters – Charge-Transfer Spectra – absolute configuration and stereochemistry of chiral metal chelates.

Unit III IR/Raman Spectroscopy

Instrumentation and Sample Handling – Characteristic vibrations – alkanes, alkenes, aromatics, alcohols, ethers phenols and amines – Carbonyl vibrations in ketones, aldehides, esters, amides, acids, anhydrides, lactones, lactams and conjugated systems – Transition metal bonds to carbonyls and other ligands - Hydrogen bonding and solvent effects – overtones, combination bands and Fermi resonance.

Unit IV Emission Spectra

Atomic Emission Spectroscopy – Spark and Arc emission – Molecular Emission – Fermi's Golden Rule – Theory of molecular Fluorescence / Phosphorescence - Typical flourophores Characteristics of flourophores - Instruments for measuring fluorescence and phosphorescence – Applications of fluorescence and phosphorescence - Chemiluminescence - Electrochemiluminescence - Distinction of luminescence and Chemiluminescence -

Unit V Miscellenous Spectral Topics

ESI-MS – Photoacoustic spectra – XPS – SEM and FESEM – TEM – Neutron diffraction

Unit VI Problems and Exercises

Recommended Books:

Resources at https://www.intechopen.com/books/

CHEM684: Molecular Magnetism and Magnetic Resonance Spectroscopy

Credits: 6

Pre-requisite: M.Sc. Chemistry or equivalent

Course Content

Unit I Magnetochemisry

Quantum theory of Para and diamagnetism – Magnetic Susceptibility and its Measurements – Spin-only formula – Organic and Main group radicals – L-S coupling – μs and μeff correlation – Time and Temperature dependence - Curie and Curie-Weiss Laws – 3d vs Heavier Analogs – Exchange coupling – Super and Antisymmetric exchange – spin crossover - Long range order - Ferro, Ferri and Antiferro coupling – anisotropy - Organic magnets – Spin glasses.

Unit II EPR Spectroscopy

Normal and Anomalous Zeeman effect – Larmor precession – Origin of EPR signal – Field modulation - Experimental setup – Radical Population – Maxwell-Boltzmann Distribution – Effective Spin Hamiltonian – First and higher order perturbations – g values – Fine structure – anisotrophy – Hyperfine and super hyperfine structures – Line widths – g and a matrices - Interpretation of radicals and single d electrons – multiple unpaired d electrons.

Unit III Basic NMR Spectroscopy

CW and FT NMR – Relaxation and NOE effects - Spectral parameters – 1H NMR Intensity, Chemical shifts, Multiplicity, and Coupling Constants - Correlation of 1H of Carbon and Hetero atoms – Chemical exchange – Deuteration effects - Virtual coupling – Stereochemistry – Hindered rotation – Karplus curves – Ring currents – Main group and Tm hydrides - Dihydrogen complexes – Double resonance and contact shift reagents – Solvent effects.

Unit IV Advanced NMR Spectroscopy

13C NMR: Proton coupled; off–resonance decoupled; proton noise decoupled 13C NMR spectra - Chemical shifts, additively effect - Chemical shifts of common organic compounds and functional groups, DEPT and SEFT spectra - NMR of common heteroatoms (N, F, O, P, S and D) - 2D NMR techniques 1H – 1H COSY, 1H – 13C COSY – HMBC, NOESY and INADEQUATE spectra – NMR imaging.

Unit V Miscellaneous Topics

NQR Spectroscopy Fundamentals – Electric Field Gradient and asymmetry – Impact of magnetic field – Spectral interpretation of Halogens, pnictogens and transition metals – Complex spectra - Mössbauer spectroscopy - Lamb–Mössbauer factor – Typical Radiation sources - spin states and splitting - Isomer shift and Quandruple splitting – Illustrative examples for Interpretation – Complications.

Unit VI Problems and Exercises

Recommended Books:

1. A. Carrington and Machlachlon, Magnetic Resonance, Harper & Row, 1967

2. R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds., John Wiley and Sons., 6th Edition.

3. W. Kemp, Organic Spectroscopy, 3rd Edition, MacMillon (1994).