DEPARTMENT OF CHEMISTRY

ISLAMIC UNIVERSITY OF SCIENCE AND TECHNOLOGY, AWANTIPORA-192122, J&K, India

Semester-III

Overview of the Course Scheme
Third Semester

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credits	Total Credits
				Internal*	Final	Total	L	T	P		
III	CHM601C	Organometallic chemistry	Core	50	50	100	3	1	0	4	26
	CHM602C	Pericylclic Reactions and Organic Photochemistry	Core	50	50	100	3	1	0	4	
	CHM603C	Electrochemistry and Solid State Chemistry	Core	50	50	100	3	1	0	4	
	CHM604C	Chemical, Thermal and Electroanalytical Methods of Analysis	Core	50	50	100	3	1	0	4	
	CHM605C	Advanced Laboratory Course	Core	50	50	100	0	0	4	4	
	CHM606E	Spectroscopy of Organic Compounds	Discipline Centric	50	50	100	3	0	0	3	
	CHM607E	Spectroscopy of Inorganic Compounds	Discipline Centric	50	50	100	3	0	0	3	
	CHM608E	Chemoinformatics	Discipline Centric	50	50	100	3	0	0	3	

*(Midterm 30 marks +Assignment 10 marks + Attendance 10 marks)

A total of 26 credits to be taken by students with following breakup:
Core = 20 Credits
Discipline Centric = 6 Credits

Third Semester
Core Course
Course Title: Organometallic Chemistry
Course code: CHM601C

Credits = 4
M.M. = 100

Unit I: Sigma bonded Organometallic Compounds

Classification, Stability, Routes of synthesis, Reactions, Structure and bonding. Decomposition pathways: α and β hydrogen transfer. Intramolecular elimination of alkane. Stability from bulky substituents, Agostic alkyls.
Metal hydride complexes: Synthesis, Characterization and Chemical reactions.

Unit II: Pi-bonded Organometallic Compounds

Classification, Synthesis, Structure and bonding in Metal-alkynes, allyIs, 1,3-butadiene and cyclobutadiene complexes
Sandwich compounds: General characteristics; Classification, Synthesis, Reactions, Structure and bonding of cyclopentadienyl complexes with special reference to ferrocene.
Compounds with transition metal—carbon multiple bonds, Alkylidene and alkylidyne synthesis, Structural characteristics, Nature of bonding.

Unit III: Catalytic Processes involving Transition Metal Organometallic Compounds
Mechanistic aspects: Oxidative addition, Insertion reactions and reductive elimination. Hydrogenation, Hydroformylation, Oxidation, Isomerization and Zeigler-Natta-- polymerization of alkenes.
C-C coupling reactions- Suzuki and Heck, Grubbs catalyst, Sonogashir, Stille couplling, Activation of small molecules like CO, CO_2 and alkanes.

Unit IV: Fluxional Organometallic Compounds
General characteristics, Rates of rearrangement and techniques of study, Classification of fluxional organometallic compounds, Some simple examples of non-rigid molecules in 4 and 5 coordination geometries, Fluxionality and dynamic equilibria in compounds such as 2-olefin, 3-allyl and dienyl complexes.

Books Recommended:

1. Principles and applications of organotransition metal chemistry, Collman J. P., Hegsdus L. S., Nortan J. R. and Finke R. G., University Science Books;1994.
2. Basic organometallic Chemistry; B. D. Gupta, A J Elias; 2nd Edn; University Press; 2013.
3. Organometallic & Bioinorganic Chemistry; Ajai Kumar; 2nd Edn ; Aaryush Education; 2016.
4. The Organometallic chemistry of the transition metals, R. H. Crabtree, John Wiley; 2014.
5. Metallo-organic chemistry, Pearson A.J., Wiley; 1994.
6. Organometallic chemistry, Mehrotra R. C. and Singh A., New Age International**; 2007.**
7. Reaction Mechanisms of Inorganic and Organometallic Systems; 3rd Edn.; Jordon; Oxford University Press; 2007.
8. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
9. Inorganic Chemistry; 4th Edn; Huheey; Harper & Row; 1990.
10. Chemistry of elements, NN Green Wood, Elsevier.

Third Semester
Core Course
Course Title: Pericyclic Reactions and Organic Photochemistry
Course Code: CHM602C

Credits = 4
M.M = 100

Unit I: Pericyclic Reactions-I

General introduction, Definition and classification of pericyclic reactions. Molecular orbital symmetry, Frontier molecular orbital concept (FMO), HOMO, LUMO and SOMO: Frontier molecular orbitals of various π-electron systems including ethene, 1, 3-butadiene, 1,3,5-hexatriene and allylic systems. Woodward Hoffman rules for pericyclic reactions.

Unit II: Pericyclic Reactions-II

Cycloadditions: Thermal and photochemical 2+2 and 4+2 cycloadditions, Suprafacial and antrafacial cycloadditions.
Electrocyclic reactions: Thermal and photochemical electrocyclic reactions of 4n and 4n+2 systems and their stereochemical aspects, Conrotatory and disrotatory motions.
Sigmatropic rearrangements: Classification, [1,3], [1,5] and [3,3] sigmatropic shifts, Cope and Claisen rearrangements, Suprafacial and antrafacial shifts of hydrogen, Biological pericyclic reactions.

Unit III: Photochemistry-I

Types of photochemical excitations, Direct and indirect excitations, The fate of excited molecule, Singlet and triplet states and their lifetimes, Jablonski diagram, Transfer of excitation energy: sensitization and quenching, quantum yield, Different types of photochemical reactions,
Photochemical reactions of alkenes: Geometrical isomerization reactions, Dimerization and cyclization reactions, Photochemical reactions of 1,3-butadiene, Rearrangements of 1,4 and 1,5-dienes, Photochemistry of vision.

Unit IV: Photochemistry-II

Photochemical reactions of saturated cyclic and acyclic carbonyl compounds, Norrish type-I and Norrish type-II reactions, Paterno-Buchi reaction.
Photochemical reactions of α, β-unsaturated carbonyl compounds (H-abstraction and isomerization to β,γ-unsaturated carbonyl compounds).
Light induced isomerizations of benzene and its alkyl derivatives, Nucleophilic photosubstitution reactions of aromatic compounds, Photo-Fries rearrangement of aryl esters and anilides. Photolysis of organic nitrites.

Books Recommended:

1. Introductory Photochemistry, A. Cox and T. Kemp McGraw Hall-1971.
2. Organic Photochemistry, 2nd Ed., J. Coxon, and B. Halton 2nd Edn .CambridgeUniversity press-1987.
3. Fundamentals of photochemistry, Rohtagi & Mukherjee Wiley Eastern-1992.
4. Advanced Organic Chemistry, Reactions, Mechanism and Structure, 4th Ed., Jerry March (Wiley, 1999).
5. Organic Chemistry, 5th Ed., John McMurry. (Brooks/Cole, 2000).
6. Organic Chemistry, J. Clayden, N. Greeves and S. Warren. Oxford University Press, 2nd Edition, 2016.
7. Pericyclic Reactions, Ian Fleming, Oxford University Press, 2nd Edition, 2015.
8. Essentials of Pericyclic and Photochemical Reactions, Biswanath Dinda, 1st Edition, 2016.

Third Semester
Core Course
Course Title: Electrochemistry and Solid State Chemistry
Course code: CHM603C

Credits = 4
M.M. = 100

Unit I: Electrochemistry-I

Ion-solvent Interactions: Non-Structural (Born) treatment and an introduction to structural (Ion-Dipole, Ion-Quadruple) treatments of ion-solvent interactions, Ion-Ion interactions: Activity and activity coefficients, Debye-Huckel theory of activity coefficients of electrolyte solutions; Derivation of Debye-Huckel limiting law, Validity and extension to high concentrations, Ion-pair formation- Bjerrum model, Debye-Huckel-Onsager conductance equation and brief idea of its extension.

Unit II: Electrochemistry-II

Metal-electrolyte electrified interfaces, Concept of surface excess, Thermodynamics of electrified interface, Lippmann equation, Electrocapillary curves, Methods for determination of surface excess. Structural models of metal-electrolyte interface: Helmholtz-Perrin, Gouy-Chapman and Stern models, Semiconductor electrodes: Structure of semiconductor/electrolyte interface, Theories of heterogeneous electron transfer: Electron transfer at electrified interface at and away from equilibrium, Butler-Volmer Equation, Low and high field approximations, Significance of transference-coefficient.

Unit III: Solid State Chemistry-I

Point groups, Space groups, Lattice Planes and Miller indices, Bragg equation, Debye-Scherrer method of X-ray structural analysis, Identification of cubic unit cells from systematic absences in diffraction pattern, Structure factor and its relation to intensity and electron density. Crystal structure of Perovskite ($SrTiO_3$) and Rutile (TiO_2).
Crystal defects and their types, Point defects: Schottky and Frenkel defects, Thermodynamics of Schottky and Frenkel defect formation, Colour centres, Dislocations and their types.

Unit IV: Solid State Chemistry-II

Band theory of solids
Semiconductors: Intrinsic and extrinsic semiconductor (n-type and p-type), Temperature dependence of charge carriers, p-n junction- devices based on p-n junction (tunnel diode, injection laser).
Super conductors: Characteristic properties- Zero resistance, Meissner effect, Heat capacity, Thermal conductivity, Absorption of electromagnetic radiations and Josephson effect. BCS theory of superconductivity, Applications.
Luminescence, Lasers: laser action, Solid state laser, Gas laser.
Liquid crystals and their applications.

Books Recommended:

1. Physical Chemistry - P. W. Atkins, Oxford, 2010.
2. Physical Electrochemistry-Fundamentals, Techniques and Applications, E. Gileadi, Wiley-VCH, 2011.
3. Electrochemistry, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH. 2nd Edn.; 2007
4. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, Ist Edn.; 2007.
5. Modern Electrochemistry 1, 2A, J. O. Bokris and A. K. Ready, Kluwer Academic/plenum Publishers, New York. 2nd Edn.; 2002,
6. Electrochemical methods, Fundamentals and Methods, A. J. Bard, L. R. Faulkner, Wiley, 2nd Edn.; 2002
7. Introduction to Solids, Azaroff, Tata McGraw,1993.
8. Solid State Chemistry and its Applications, A R West, Wiley,1989.
9. Solid State Physics, N.W.Ashcroft and N.D.Mermin, Saunders College, 2001.
10. Elements of Solid state Physics, J.P. Srivastava, Prentice Hall of India, 2003.

Third Semester
Core Course
Course Title: Chemical, Thermal and Electroanalytical Methods of Analysis
Course Code: CHM604C

Credits = 4
M.M. = 100

Unit I: Acid Base Titrations

Titrations in Analytical chemistry. Titration curves for strong acid- strong base, weak acid- strong base and weak base-strong acid titrations, Polyfunctional acids and bases. Determining the equivalence points, Theory of acid- base indicator, selection of proper indicator, indicator errors. Determination of nitrogen, sulphur, ammonium salts, nitrates and nitrites, carbonates and bicarbonates and other organic functional.

Titrations in non-aqueous solvents, Solvents for non-aqueous titrations, indicators for non-aqueous titrations, characteristics of amphiprotic solvents-Autoprotolysis, Aprotic solvents, choosing a solvent. Some selected solvents, titrants and standards, effect of water. Determining the equivalence point. Typical applications, Determination of carboxylic acid, phenols, and amines.

Unit II: Complexation Titrations

Introduction, Types of EDTA titration (Direct, back, replacement and other miscellaneous methods), Formation of complexes. Complexation equilibrium, Complexation Titration, stability of complexes, stepwise formation constants, chelating agents. Aminocarboxylic acid titrations, complexes with metal ions, equilibrium calculations involving EDTA, Factors affecting the shape of EDTA titration curves. Completeness of reactions, indicators for EDTA titrations, theory of common indicators.

Precipitation titrations: Titration curves feasibility of precipitation titrations. Factors affecting shape- titrant and analyte concentration. Completeness of the reaction. Titrants and standards. Indicators for precipitation titrations involving silver nitrate. Volhard, Mohr and Fajan's methods. Typical applications.

Unit III: Thermal Methods of Analysis

Introduction to thermal methods of analysis, Thermo gravimetric analysis (TGA), Apparatus, Methodology, Factors effecting TGA curve, Applications of TGA for quantitative analysis, thermal stability of materials, mixture analysis, Kinetic studies, (TG analysis of $CaC_2O_4.H_2O$, $CuSO_4.5H_2O$, problems based TGA)

Differential thermal analysis (DTA), Apparatus, Methodology, simultaneous DTA and TGA curves, Interpretation of TGA and DTA curves of compounds e.g., Calcium oxalate monohydrate, Magnesium oxalate monohydrate,

Brief introduction to Thermometric titrimetric and applications to acid-base and complexometric titrations.

Unit IV: Electrochemical Methods

Voltametry and polarographic analysis: Principle of polarography, residual current, migration current, diffusion current, half wave potential, Ilkovic equation, instrumentation, Dropping mercury electrode (DME), Advantages and dis-advantages of DME, Qualitative and quantitative analysis of inorganic ions Cu, Bi, Pb, Cd, Zn, AC polarography, Pulse polarography Anode stripping voltametry: Principle, instrumentation, Hanging mercury drop electrode, Application in the analysis of Pb and Cd in environmental samples, Principle of cathode stripping voltammetry

Books Recommended:

1. Principals of Physical chemistry, Puri, Sharma , Pathania, 4th edition 2016-17
2. Ionic Equilibria in Analytical Chemistry; Freiser and Fernando, 1966.
3. Introduction to chemical Analysis, R. D.Braun, Mc. Graw-Hill, International Book Co., 1983
4. Chemical Analysis, 2nd Ed., H.A. Laitinen and W.E. Harris, McGraw Hill Kogakusha, Ltd., 1975.
5. Instrumental Methods of Analysis, 7th Ed., Willard, Merritt, Dean and Settle, CBS Publishers, New Delhi.
6. Instrumental methods of Chemical Analysis, 5th edn., G.W. Ewig, McGraw Hill Book Co., 1985.
7. Instrumental Methods of Analysis by G.D. Christian and C.N. Reilly. 2nd Edn.; 1986.
8. Principle of Instrumental Methods of Analysis; D.A. Skoog. D.M. West and F.J. Holler, Sounders College Publishing New York, 2001.

Third Semester
Core Course
Course Title: Advanced Laboratory Course
Course Code: **CHM605C**

Credits = 4
M.M. = 100

Spectrophotometry

1. To study the complexation reaction between Fe (III) & salicylic acid.
2. Determine the dissociation constant of an indicator by spectrophotometric method.
3. Determination of Iron (II) with 1,10-Phenanthroline.
4. Determination of Phosphate by Molybdenum blue method.
5. Estimation of aspirin from given tablet by Spectrophotometry
6. Interpretation of IR spectrum of alcohols, ketones, aldehydes and other standard material

Potentiometry

7. Precipitation titration of KCl, KBr, KI and their mixture with $AgNO_3$
8. Determination of formation constant of Ag-NH_3 complex
9. Standardization of an Iron (II) solution with a standard dichromate solution over Pt & Calomel assembly.
10. Estimation of iodide with Standard $AgNO_3$ over Pt and Calomel assembly using I^-/ I_2 redox couple.
11. Simultaneous determinations of chloride and iodide ions with Standard $AgNO_3$ over Ag-Glass electrode assembly

Conductometry

12. Verification of Debye-Huckel-Onsagar law.
13. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ in a mixture.
14. To determine the solubility and solubility product of a sparingly soluble salt ($BaSO_4$) in water.
15. To determine the basicity of sodium potassium tartarate by conductometric method.

Kinetics

16. Study the kinetics of reaction between potassium persulphate and potassium iodide:
    a) Determine the rate constant and order of reaction.
    b) Study the influence of ionic strength on the rate constant.

Viscometry

17. Determination of Mol. Mass of a Polymer (Polyvinyl alchol) using viscosity method.

Polarimetery

18. Determination of specific, molecular and intrinsic rotation of an optically active compound
19. Study of inversion of cane sugar in presence of acid.

pH-metric Titrations

20. Purity of Acetyl Salicylic acid (Aspirin) in a commercial tablet by pH Titration.
21. Quantitative analysis of chromate dichromate mixture by pH titration.

Flame Photometry

22. Simultaneous determination of sodium and potassium in a given mixture
23. Determination of cadmium and magnesium in tap water

Chromatography

24. Separation of some organic compounds by column chromatography
25. Analysis of Paracetamol from given unknown sample by HPLC
26. Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.

27. Separation of two Cobalt (III) complexes viz $[Co(NH_3)_6]Cl_3$ and $[Co(NH_3)_5Cl]Cl_2$ on Silica column.

Synthetic Preparations

28. Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.
29. Preparation of trans dicholoro bis (ethylenediamine), cobalt (III) chloride and its conversion to cis-isomer.
30. Reaction of Cr(III) with a multidentate ligand; a kinetic experiment (visible spectra Cr-EDTA complex)
31. Synthesis of aspirin and its characterization by physical and spectroscopic methods.
32. Synthesis of paracetamol and its characterization by physical and spectroscopic methods.
33. Beckmann rearrangement.

Extraction/Estimation of Organic compounds from natural sources

34. Isolation of lycopene and beta-carotene from tomato, Characterization of lycopene/P-carotene by UV -absorption process.
35. Isolation of caffeine from cold drinks and its physicochemical analysis.
36. Estimation of ascorbic acid in Vitamin C tablet by titration with potassium bromate
37. Estimation of phosphoric acid in soft drink by molybdenum blue method.
38. Estimation of BOD and DO in Waste Water Sample
39. Estimation of acid value of oil

Books Recommended:

1. Practical Physical Chemistry ----Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. ---- Schoemaker et al. (MGH, 2003)
4. Synthesis and Technique in Inorganic ch mnbhyy chemistry , G. S.Girlomi; R.J. Angleci 3rd edn.; University Science Books.
5. Synthesis and characterization of Inorganic compounds W.AJolly
6.Experimental Inorganic / Physical Chemistry ; Mounir A. Malati Horwood/1999.
7. Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
8. Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ; 1995.
9. Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books 2002.
10. Practical Clinical biochemistry methods and interpretations, R.Chawla, J.P. Bothers Medical Publishers (P) ltd., 1995.
11. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
12. Practical clinical Biochemistry-Harold Varley and Arnold.Hein mann, 4th edn
13. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint.2003 Pearson Education Pvt. Ltd., New Delhi
14. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 Prentice Hall, Inc. New Delhi.
15. Quantitative Chemical Analysis; Kolthoff, sandell Meehan and Bruckestein; Mcmillan Co., London, 1969

Third Semester
Discipline Centric Course
Course Title: Spectroscopy of Organic Compounds
Course Code: CHM606E

Credits = 3
M.M = 100

Unit I: Ultraviolet and Infrared Spectroscopy

Introduction, Ultraviolet absorption spectra of dienes (homo and heteroannular), Enones, Carbonyl compounds, Unsaturated carbonyl compounds, Aromatic and heteroaromatic compounds, Effect of solvent on electronic transitions, Effect of conjugation on ultraviolet spectra, Woodward-Fieser rules, Applications and limitations, Kuhn's rule, Application to conjugated polyenes.
Introduction, Characteristic vibrational frequencies of alkanes, Alkenes, Alkynes, Alcohols, Ethers, Phenols, Amines, Aldehydes, Ketones, Acids, Anhydrides, Esters, Lactones, Amides and conjugated carbonyl compounds, Effect of hydrogen bonding and solvent on vibrational frequencies in IR spectra.

Unit II: Mass Spectrometry

Introduction, Instrumentation, A typical mass spectra, molecular ion peak, Ion production, EI, CI, FD, FAB, ESI and MS/MS methods, Role of isotopes in mass spectrometry, Fragmentation pattern of various classes of organic compounds, Metastable peak, Nitrogen rule, High resolution mass spectrometery. Fragmentation pattern, Initial ionization event, α-cleavage, Inductive cleavage, Two bond cleavage, Retro-Diels Alder cleavage and McLafferty rearrangement.

Unit III: Proton Nuclear magnetic resonance spectroscopy (^{1}H-NMR)

Shielding effect, Chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (Alcohols, Phenols, Enols, Carboxylic acids, Amines, Amides and mercapto). Chemical exchange, Effect of deuteration, Complex spin-spin interactions between two three, four and five nuclei (first order spectra) virtual coupling, Stereochemistry. Simplification of complex spectra, Nuclear magnetic double resonance, Contact shift reagents, Solvent effect, Fourier transform technique, Nuclear overhauser effect (NOE). Bio-chemical applications of NMR (examples).

Unit IV: Carbon-13 NMR Spectroscopy

General considerations, Chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromtic and carbonyl carbon), Coupling constant, Two dimensional NMR spectroscopy (brief idea)- COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques. Problems on structure elucidation based on the data from different spectroscopic techniques.

Books recommended:

1. Spectroscopy of Organic Compounds, P.S. Kalsi, New Age International Private Limited (1 January 2016).
2. Introduction to Spectroscopy. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan. Cengage Learning, 2008.
3. Spectrometric identification of Organic Compounds.5th Ed., R. M. Silverstein, G. C. Bassler and T. C. Morill. (Jhon Wiley-1991).
4. Introduction to NMR Spectroscopy, R. J. Abraham. J. Fisher and P. Loftus (Wiley- 1991)
5. Applications of absorption spectroscopy of Organic Compounds, J. R. Dyer (Prentice Hall-1991).
6. Spectroscopic Methods in organic Chemistry, D. H. Williams; I. Fleming (Tata- McGraw Hill-1988).

Third Semester
Discipline Centric Course
Course Title: Spectroscopy of Inorganic Compounds
Course Code: CHM607E

Credits = 3
M.M. = 100

Unit I: NMR Spectroscopy

Multinuclear NMR spectroscopy in inorganic chemistry. Paramagnetic shift in ^{1}H NMR spectra, ^{31}P NMR, ^{11}B NMR ^{19}F NMR (Splitting pattern and spectrum). Exchange process in solution Spin-spin coupling, Magnetic resonance imaging (MRI), MRI contrast agents, Brief introduction of solid-state NMR.

Unit II: Mossbauer Spectroscopy (MB Spectroscopy)

Technique of Mossbauer Spectroscopy, Gamma-ray fluorescence, Gamma radiation source, Doppler effect, Isomer shift, quadrupole splitting, Magnetic hyperfine splitting, Applications in inorganic complexes (Bonding and Structure of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+}, Recognition of nature of M-L bond, Coordination compound, Structure and oxidation state.

Unit III: Electron Spin Resonance (ESR/EPR Spectroscopy)

Principle of ESR spectroscopy. Hyperfine structure in ESR spectra, Hydrogen atom, Methyl radical, $(SO_3)_2NO^-$ anion, Fermi-contact interaction, *g*-factor: g_{11} *and* $g_{\perp}$. Applications of ESR, Spin labels, McConnell equation, Isotropic and anisotropic systems, Hyperfine splitting, Spin hamiltonian, Kramer's degeneracy and Zero field splitting. ESR Spectra of some transition metal complexes and biomolecules.

Unit IV: Nuclear Quadrupole spectroscopy (NQR)

NQR Isotopes, Basic theory of quadrupole spectroscopy, Quadrupole nuclei, Nuclear quadrupole moment, Electric field gradient (EFG), Nuclear Quadrupole Coupling constant, Effect of applied magnetic field (Zeeman effect), Towns-Dailey Theory, Applications of NQR and NQR spectra of $^{14}N_7$, $^{11}B_5$.

Books Recommended:

1. NMR, NQR and EPR and Mossbauer Spectroscopy in Inorganic Chemistry; Parish and Elis, H; 1990.
2. Nuclear Quadrupole Resonance Spectroscopy, Das, T. P. and Hahn, E. L. Academic Press; 1958.
3. Principles of Physical Chemistry; Pure, B. R. Sharma, L. R. and Pathiana, M. S; 47th Edition.
4. Spectroscopy in Inorganic Chemistry; Vol I and II; Rao, Ferraro; Academic Press; 1970.
5. Structural Methods in Inorganic Chemistry; 2nd edn; Ebsworth, E. A. V and Rankin, D. W. H; ELBS; 1991.
6. Inorganic Chemistry; Catherine, E. H and Sharpe, A. G; 2nd Edition, Pearson.

Third Semester
Discipline Centric Course
Course Title: Chemoinformatics
Course code: CHM608E

Credits = 3
M.M. = 100

Unit I: Representation of Molecules and Chemical Reactions

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Unit II: Searching Chemical Structure

Full structure search, sub structure search, basic ideas, similarity search, Three dimensional search methods, Basics of computation of physical and chemical data and structure descriptors, Data visualization.

Unit III: Computer Assisted Virtual Screening Design

Structure based virtual screening- Protein ligand docking, Scoring functions for protein ligand docking, Practical aspects of structure based virtual screening, Prediction of ADMET properties, 2 D and 3D data searching, Chemical databases, Role of computers in chemical research.

Unit IV: Application of Chem-informatics in Drug Design

Quantitative structure-property relations,
Descriptor analysis, Computer assisted structure elucidations, Target identification and validation, Lead finding and optimization, Analysis of HTS data, Design of combinatorial libraries, Ligand and structure based drug design

Books Recommended:

1 Andrew R. Leach, Valerie J. Gillet, Cluwer , Introduction to Chem-informatics, Academic Publisher, Netherlands, 2003
2. Lisa B. English (Editor), Combinatorial Library Methods and Protocols, Humana Press Inc, Volume:201, 2002
3. Frank Jensen, Introduction to Computational Chemistry, Wiley Publisher, Second Edition, 2006