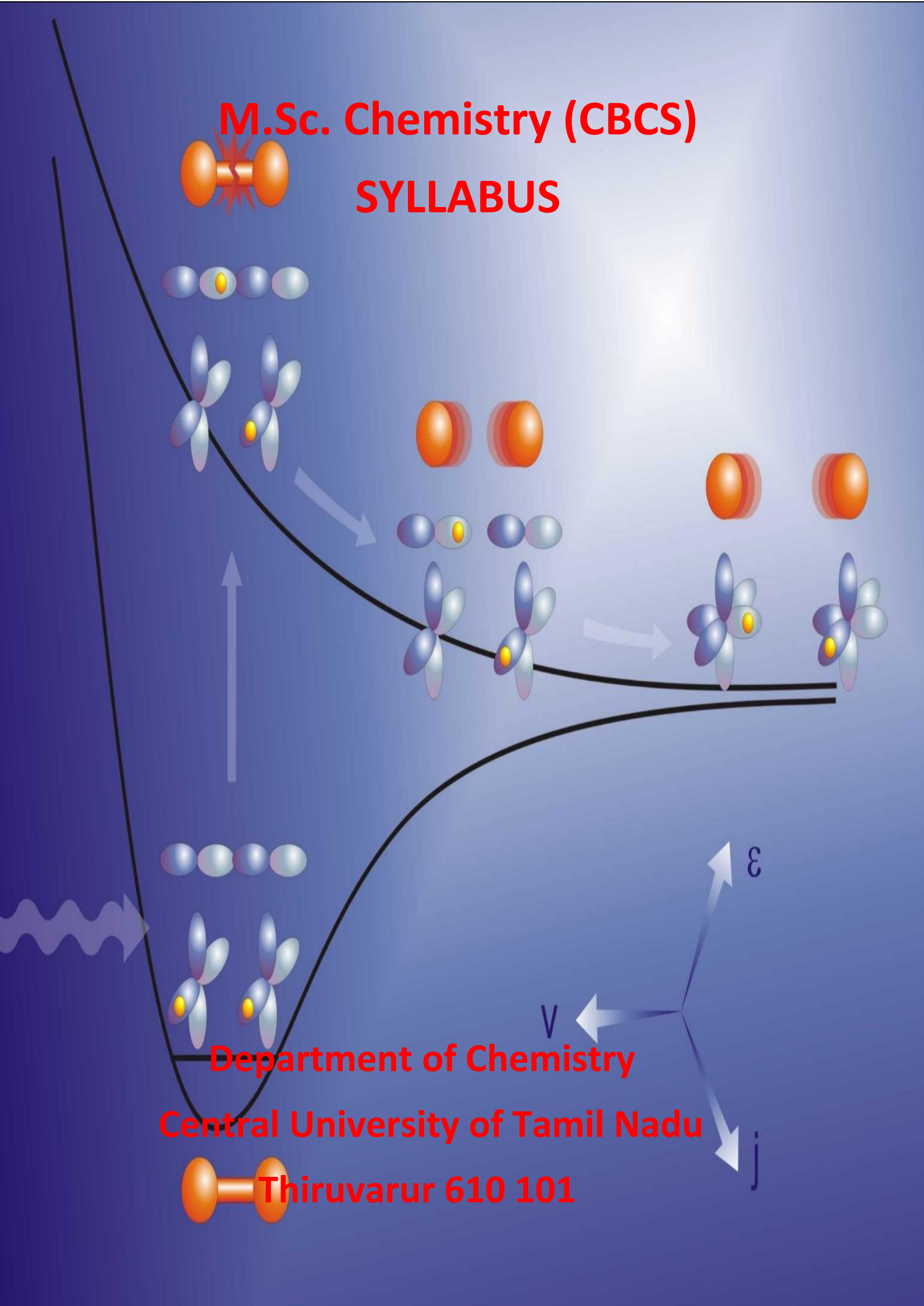
M.Sc. Chemistry (CBCS)

SYLLABUS



Department of Chemistry

Central University of Tamil Nadu

Thiruvarur 610 101

Name of the course	:	**M. Sc. (Chemistry)**
Duration	:	4 semesters
Intake	:	16
Eligibility	:	Bachelor's degree in Chemistry (Main) or with Chemistry as one of the major subjects. Candidates should have secured a minimum of 60% marks or 6.5 CGPA (on a 10- point scale) in the qualifying degree examination for General category, 55% marks or 6.0 CGPA (on a 10 point scale) for OBC and 50% aggregate marks or 5.5 CGPA (on a 10-point scale) for SC/ST candidates. The candidates should not have completed 24 years.

Contents and Credits

Course Code	Title of the Course	Credits
CH0101	Crystal Packing and Coordination Chemistry	4
CH0102	Stereochemistry, Aromaticity and Heterocycles	4
CH0103	Quantum Chemistry and Group Theory	4
CH0104	Advanced Organic Chemistry Laboratory I	3
CYE* **	**ELECTIVE - I**	**3**
CYE* **	**ELECTIVE - II**	**3**
CH0201	Organometallics, catalysis and spectroscopy	4
CH0202	Photochemistry, Pericyclics and Rearrangements	4
CH0203	Quantum Chemistry and Molecular Spectroscopy	4
CH0204	Physical methods in Chemistry	4
CH0205	Advanced Physical Chemistry Laboratory I	3
CYE* **	**ELECTIVE - III**	**3**
CH0301	Bio-Inorganic Chemistry And Inner Transition Elements	4
CH0302	Advanced Organic Chemistry III	4
CH0303	Statistical Thermodynamics, Chemical Kinetics and Electrochemistry	4
CH0304	Advanced Inorganic Chemistry Laboratory I	3
CYE* **	**ELECTIVE - IV**	**3**
CYE* **	**ELECTIVE - V**	**3**
CH0401	Research Project	6
CYE* **	**ELECTIVE - VI**	**3**
TOTAL CREDITS		**73**

Semester: 1 **Subject Code: CH0101** **Credits: 4** **4-0-0-4**

Title: Crystal Packing and Coordination Chemistry

Specific objectives:

To introduce the inorganic chemistry concepts and the properties of the main group elements, basic coordination chemistry and inorganic photochemistry.

Learning outcomes:

Ensures the students to understand, concepts and the properties of the main group elements, basic coordination chemistry and inorganic photochemistry.

Pre-requisite:

Inorganic Chemistry, periodic properties.

Syllabus:

The Chemistry of the Main Group Elements: Inorganic Rings, chains and cages - Catenation and Heterocatenation, Heterocyclic ring system- Borazines, Phosphazines-Monomer and Polymer, S-N ring compounds, Homocyclic rings of S, Se and Te. Silicate minerals, Isopolyanions, Boranes: boron cage compounds-*closo*, *nido*, *arachno*, carboranes; cage compounds of S and P.

Advanced Solid State Chemistry: Ionic solids, close packing, radius ratio rules, Structures of ionic crystals – AX and AX_2 type crystal structures – layer structures - lattice energy - Born-Lande, Born-Mayer and Kapustinskii equations – Derivations and applications – Decomposition of ionic solids – solubility of ionic solids. Defects and Non-stoichiometric - Intrinsic and extrinsic defects - point, line and plane defects; vacancies, Stoichiometric defects - Schottky and Frenkel defects - Non-stoichiometry – Metal excess and Metal-deficiency. Thermodynamic and structural aspects. n- And p- type semiconductors–photovoltaic cell – Superconductivity.

Theories of Metal-Ligand Bond: VB theory and its limitations – crystal field theory - splitting of d-orbitals under various geometries – factors affecting splitting – CFSE and evidences for CFSE (Structural and thermodynamic effects) – Spectrochemical series – Jahn-Teller distortion - site preferences - limitations of CFT – ligand field theory – MO theory – sigma – and pi-bonding in complexes and evidences for pi-bonding – nephelauxetic effect – angular overlap model.

Coordination Chemistry – Reaction Mechanism: Kinetics and mechanism of reactions in solution – labile and inert complexes – ligand displacement reactions in octahedral and square planar complexes – acid hydrolysis, base hydrolysis and anation reactions – trans effect – theory and applications. Electron transfer reactions – complementary and non-complementary types – inner sphere and outer sphere processes – Excited state outer sphere electron transfer reactions - isomerisation and racemisation reactions of complexes – reactions of four and six-coordinate complexes – interconversion between stereoisomers.

Prescribed Books

1. Huheey J. E., Keiter E. A. and Keiter R. L. and Medhi O. K., *Inorganic Chemistry - Principles of Structure and Reactivity*, 4th edition, Pearson Education, **2006**.
2. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.
3. B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of* 3rd *Inorganic Chemistry*, 3rd edition, John Wiley & Sons, **2010**.
4. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, ed., Wiley-Eastern Company, New Delhi, **1990**.
5. Azaroff, L.V., Introduction to Solids, McGraw hill, New York. **1960**
6. West, A. R., Solid State Chemistry and Its Applications, John Wiley & Sons, **1984**.
7. Chakrabarty, K., Solid State Chemistry, New Age Publishers, **1996.**
8. Keer, H. V., Principles of the Solid State, Wiley Eastern Limited, **1993**.

Reference Books

1. Day, M. C., and Selbin, J., *Theoretical Inorganic Chemistry*, Affiliated East West Press Pvt. Ltd. 2nd edition, **1985**.
2. Kettle, S. F. A., Physical Inorganic Chemistry – *A Coordination Chemistry Approach*, Spectrum Academic Publishers, Oxford University Press, **1996**.
3. Basolo, F., and Pearson, R. G., *Mechanism of Inorganic Reactions*, John Wiley, New York, **1967**.
4. Miessler, G. L., and Tarr, D. A., *Inorganic Chemistry*, 3rd edition, Pearson, **2004**.
5. Housecraft, C. E., and Alan G. Sharpe, *Inorganic Chemistry*, 4th edition, Pearson, **2012**.
6. Purcell, K. F., and Kotz, J. C., *Inorganic Chemistry*, Cengage Learning, **2012**.
7. Day Jr ,M. C., and Selbin, J, *Theoretical Inorganic Chemistry*, Literary Licensing, LLC, **2012**
8. Wilkinson, G., Gillars, R. D., and Mccleverty, J. A., *Comprehensive Co-ordination Chemistry*, Pergamon Press, **1987**.
9. Wulfberg, G., *Inorganic Chemistry*, University Science Books, **2000**.

Semester: 1 **Subject Code: CH0102** **Credits: 4** **4-0-0-4**

Title: Stereochemistry, Aromaticity and Heterocycles

Specific objectives:

To introduce advanced level study in stereochemistry, aromaticity, heterocyclics and physical organic chemistry.

Learning outcomes:

Ensures the students to understand, acquire knowledge on topicity, asymmetric synthesis, determining the reaction mechanisms by different methods, criteria for aromaticity in non- benzenoid molecules and other advanced polycyclic aromatics and the nomenclature and reactions of complex heterocyclics.

Pre-requisite:

Basics in stereochemistry and physical organic chemistry.

Syllabus:

Advanced Stereochemistry: Configuration - conformation of cycloalkanes, conformation and reactivity -stereochemistry of allenes, spiranes, biphenyls, molecules with chiral planes, Topicity stereoselective and stereospecific reactions - enantioselective reactions - double stereo differentiation, asymmetric synthesis, chiral auxiliaries, chiral catalysts and reagents.

Introductory physical organic chemistry: Thermodynamic stability – general relationship between thermodynamic stability and reaction rates – electronic substituent effects on reaction intermediates – kinetic isotope effects – linear free energy relationships – principles of microscopic reversibility – substituent effects – solvent and solvent effects – methods of determination of reaction mechanism.

Aromaticity: Criteria of aromaticity - Craig's rule – non-benzenoid aromatic compounds – anti-aromaticity, homo aromaticity – fused-ring systems – hetero aromatic systems.

Nucleophilic aromatic substitution reactions – VNS - transition metal- catalyzed aromatic substitution reactions – aromatic substitution reactions involving radical intermediates.

Advanced Heterocycles: Nomenclature, heterocyclics with two hetero atoms – fused five and six membered heterocyclics – preparation and reactions of indole, quinoline, isoquinoline and carbozole.

Prescribed books:

1. Nasipuri, D., *Stereochemistry* of Organic Compounds: Principles and Applications, 4th edition, New Academic Science Publisher. **2012**.

2. Eliel, E. L., and Wilen, S. H. Stereochemistry of Organic Compounds, Wiley, **1994**.
3. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edition, **2007**.
4. Heterocyclic Chemistry- J. A. Joule, K. Mills, G. F. Smith, Blackwell publishing Ltd, 5th edition, **2010.**

Reference books:

1. Morrison, R. T., Boyd, R. N. and Bhattacharjee, S. K., Organic Chemistry, 7th edition, Pearson Prentice Hall, **2011**.
2. Pine, S. H., Organic Chemistry, Tata McGraw Hill, 5th edition, **2008**.
3. Carruthers, W., and Coldham, I., Modern methods of Organic Synthesis, Cambridge University Press, First South Asian edition, **2005**.
4. J. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th edition, Wiley, **2007**.

Semester: 1 **Subject Code: CH0103** **Credits: 4** **4-0-0-4**

Title: Quantum Chemistry and Group Theory

Specific objectives:

To introduce Quantum chemistry, molecular symmetry and point groups for various molecules.

Learning outcomes:

Ensures the students to understand, acquire knowledge in quantum chemistry and group theory symmetry.

Pre-requisite:

Basic mathematics and physics at the iMSc I/II year levels. Preliminary knowledge of symmetry and group

Syllabus:

Quantum Chemistry I: Classical mechanics, black body radiation, uncertainty principle and wave particle duality, wave equation, wave functions, properties of wave functions, Normalization of wave functions, orthogonality of wave functions, one dimensional wave equation, separation of variables for solving wave equation, general solutions to wave equations, two dimensional wave equations.

Postulates of quantum mechanics, Wave function of a particle - Schrödinger equation, Eigen value problem, linear operator's classical mechanical quantities in quantum mechanics, wave function normalization, Particle in one dimensional and three dimensional box, Harmonic oscillator.

Group Theory: A systematic procedure for symmetry classification of molecules. Symmetry elements, symmetry operations, concepts of groups, Sub-groups, classes of symmetry operations, group multiplication tables. Abelian and non-Abelian point groups. symmetry criterion of optical activity, symmetry restrictions on dipole moment, representation of groups, matrix representation of symmetry operations, reducible and irreducible representations, application of orthogonality theorem.

Construction of character tables for point groups C2v, C3v and D2h, structure of character

Tables, determination of symmetry species for translations and rotations.

Atomic term symbols and electronic configuration for multi electron systems, Russel-Saunders coupling, J-J coupling.

Prescribed Books

1. Cotton, F. A.; *Chemical Applications of Group Theory*, John Wiley & Sons Inc., 3rd edition, **2009.**
2. Veera Reddy, K., *Symmetry and spectroscopy of molecules*, New Age International, 2nd edition, **2009**
3. McQuarie, D.; *Quantum chemistry*, University Science Publishers, **2007.**
4. McQuarie, D. A.; Simon, J. D.; *Physical Chemistry: A Molecular Approach*, University Science Books, **2011.**

Reference Books

1. Jaffe, H. H.; Orchin, M.; Symmetry in Chemistry, John Wiley & Sons Inc., **2002**.
2. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.
3. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6th edition, **2008.**
4. Raff, L. M.; Principles of Physical Chemistry, Prentice Hall, **2001.**
5. I. N. Levine, Molecular Spectroscopy, John Wiley, **1975.**
6. Harris, D. C.; Bertolucci, M. D.; Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy, Dover Publications, **1989.**
7. Lowe, J. P., Peterson, K.A., Quantum Chemistry, Academic press, **2011**.

Semester: 1 **Subject Code: CH0104** **Credits: 3** **0-1-5-3**

Title: Advanced Organic Chemistry Laboratory I

Specific objectives:

To introduce multistep organic synthesis and its spectroscopic analysis, separation and estimation of organic compounds.

Learning outcomes:

Ensures the students to understand, acquire knowledge and have hands on experience in multistep organic synthesis and analysis by using spectroscopic techniques. Separation techniques and functional group analysis.

Pre-requisite:

Single step preparations

Syllabus:

Multistep organic synthesis- conventional synthesis - microwave assisted synthesis - photochemical reactions. Purification of the compounds using column chromatography and characterization of the compounds using MS, IR, ^{1}H and ^{13}C NMR techniques.

Qualitative Analysis: Separation and analysis of organic mixture containing two components and preparation of suitable derivatives.

Reference Books

1. Singh, P. R., Gupta, D. S., Bajpai, K. S., Experimental Organic Chemistry Vol 1 and 2, Tata McGraw Hill
2. Bansal, R. K., Laboratory Manual in Organic Chemistry, Wiley, **2006**.
3. Vogel , A.I., Tatchell, A.R., Furnis , B.S., Hannaford , A.J., Smith, P.W.G., Vogel's Practical Organic Chemistry, 5th edition, Pearson education Ltd, **1996**.

Reference Books:

1. Leonard, J., Lygo, B., Procter, G., Advanced Practical Organic Chemistry, 3rd edition, CRC press, **2013**.
2. Singh, P. R., Gupta, D. S., Bajpai, K. S., Experimental Organic Chemistry Vol 1 and 2, Tata McGraw Hill
3. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley. **2006**.
4. Silverstein, R. M. and Webster, F. X., Spectrometric identification of organic compounds, John Wiley and Sons.Inc. , 6th edition, **1997**.

Semester: 2 **Subject Code: CH0201** **Credits: 4** **4-0-0-4**

Title: Organometallics, Catalysis and Spectroscopy

Specific objectives:

To introduce the concepts of organometallics, bonding, structure, reaction mechanism, catalysis and spectroscopy to study them

Learning outcomes:

Ensures the students to understand, acquire knowledge on ligands and fluxional molecules, different organic ligands and metal complexes, reaction mechanism, catalysis and spectroscopic techniques.

Pre-requisite:

Basic inorganic chemistry

Syllabus:

Structure and bonding in organometallics: 18-Electron rule - metal carbonyls – bonding – spectra – metal alkyls, aryls, hydrides and dihydrogen complexes - ligands – metallocenes - electronic structure and bonding in ferrocene - synthesis, physical and spectroscopic properties of metallocenes – fluxional molecules.σ–bonded ligands: metal- phosphines / metal- nitrosyls: structures, reactivity and bonding. Carbenes: N-heterocyclic carbenes, Fischer carbenes, Schrock carbenes, carbynes. Isolobal analogy, metal-metal bond, transition metal clusters.

Reaction mechanism and catalysis: oxidative addition, reductive elimination, insertion, hydride elimination, abstraction; hydrogenation of olefins, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, Isomerization reactions, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation, carbonylation, and CH functionalization reactions. Applications of organometallics in organic synthesis: C-C coupling reactions (Heck, Sonogoshira, Suzuki etc).C-N bond coupling reactions and asymmetric hydrogenations.

Electronic Spectroscopy: Microstates, - terms and energy levels for d^1 - d^9 ions in cubic and square fields – Intensity of bands – group theoretical approach to selection rules - Effect of distortion and spin-orbit coupling on spectra- Orgel and Tanabe-Sugano diagrams – Evaluation of 10Dq and β for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra – electronic spectra of

$[Ru(bipy)_3]^{2+}$. Optical rotatory dispersion, circular dichroism and Magnetic circular dichroism – applications to metal complexes.

Infrared and Raman Spectroscopy: Vibrations in simple molecules (H_2O, CO_2) and their symmetry notation for molecular vibrations – combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules - effect of coordination on ligand vibrations – uses of groups vibrations in the structural elucidation of metal complexes. Applications of IR and Raman spectroscopy to inorganic compounds.

Prescribed Books

1. Powell, P., *Principles of Organometallic Chemistry*, 2nd ed., Springer, **1998**.
2. Purcell, K. F., and Kotz, J. C., *Inorganic Chemistry*, Saunders Golden Sunburst Series, W. B. Saunders Company, Philadelphia, **1977**.
3. Huheey, J. E., Keiter, E. A. and Keiter, R. L. and Medhi, O. K., *Inorganic Chemistry - Principles of Structure and Reactivity*,4th edition, Pearson Education, **2006**.
4. Mehrotra, R. C., and Singh, A., Organometallic Chemistry, a Unified Approach, New Age International, **2006**.
5. Crabtree, R. H., *Organometallic Chemistry of the Transition Metals*, Wiley, New York, **1988**.
6. Gupta, B. D., and Elias, Anil. J., Basic Organometallic Chemistry: Concepts, Syntheses, and Applications of Transition Metals, 1st edition, Universities Press, CRC Press, **2010**.
7. Drago, R. S., *Physical Methods for Chemistry*, 2nd edition, Saunders College Publishing, **1992**.
8. Lever, A. B. P., *Inorganic Electronic Spectroscopy*, 2nd Sub. Edition, Elsevier Science, **1986**.

Reference Books

1. Elschenbroich, C., and Salzer, A., *Organometallics: A Concise Introduction*, 3rd edition, **1999**.
2. Greenwood, N. N., and Earnshaw, A., *Chemistry of the Elements*, 2nd edition, Elsevier, **2005**.
3. Jolly, W. L., *Modern Inorganic Chemistry*, McGraw Hill, New York, 2nd Edition, **1991**.
4. Douglas, B., McDaniel, D, .and Alexander, J., *Concepts and Models of Inorganic Chemistry*, John Wiley, New York, 3rdedition., **1993**.
5. Kegley, S. E., and Pinhas, A. R., *Problems and Solutions in Organometallic Chemistry*, University Science Books, Oxford University Press, **1986**.
6. Douglas, B., McDaniel, D. H., and Alexander, J. J., Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley & sons, New York, **2006**.
7. Bochmann, M., Organometallics 1: Complexes with transition metal-carbon s-bonds;
8. Oxford Chemistry Primers Series,No. 13 Oxford Chemistry Primers Series, No. 12, **1994**.; Bochmann, M., Organometallics 2:Complexes with transition metal-carbon p-bonds, **1994.**
9. Collman, J. P., Hegedus, L. S., Nortan, J. R. and Finke, R. G., Principles and Applications of Organotransition Metal Chemistry, University Science Books. Mill Valley, California, **1987**.

Semester: 2 **Subject Code: CH0202** **Credits: 4** **4-0-0-4**

Title: Photochemistry, Pericyclics and Rearrangements

Specific objectives:

To introduce the concepts of photochemistry, pericyclics, rearrangements and name reactions.

Learning outcomes:

Ensures the students to understand, acquire knowledge on Pericyclic reactions, organic photochemistry, molecular rearrangement and name reactions and their further applications in organic synthesis.

Pre-requisite:

Basic organic chemistry

Syllabus:

Pericyclic Reactions: Pericyclic reactions – orbital correlation diagram – FMO. Diels-Alder reactions – 1,3-dipolar cycloaddition reactions – [2+2] cycloadditions and related reactions leading to cylcobutanes – [3,3] and [2,3]-sigmatropic rearrangements –unimolecular thermal elimination reactions.

Organic photochemistry: Photochemistry of alkenes, dienes and polyenes – photochemistry of carbonyl compounds – photoreductions, photooxidations and photorearrangement reactions - photochemistry of aromatic compounds.

Molecular Rearrangements: Classification – electrophilic, nucleophilic and free radical rearrangements, mechanisms of the following rearrangements – pinacol – pinacolone, Wagner – Meerwin, Tiffenev-Demjanov, Dienone- Phenol, Favorskii, Hofmann, Schmidt, Lossen, Curtius, Beckmann, Fries, Baeyer – Villager, Stevens, Benzil – Benzilic acid, Brook and Benzidine, sommelet hauser rearrangement, rearrangements.

Selected name reactions in organic synthesis: Wittig Reaction, Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction, nazarov cyclization.

Prescribed books

1. Carey F.A., and Sundberg, R.J., Advanced Organic Chemistry, Part B: Reactions and synthesis, 5th edition, **2007**.
2. Fleming, Pericyclic Reactions, Oxford University Press, Oxford, **1999**.

3. Mukherjee, S.M. and Singh, S.P., Pericyclic Reactions, MacMillan India, New Delhi.
4. Sankararaman, S., Pericyclic Reactions - Applications and Theory, Wiley – VCH, **2005**.
5. Turro, N. J., Scaiano, J. C., and Ramamurthy, V., Modern Molecular Photochemistry of Organic Molecules, University Science Books, **2010.**
6. Sanyal and Sanyal, Reactions, Rearrangements and Reagents, Bharati Bhawan Publishers & Distributors; 4th edition, **2003**

Reference books

1. Morrison, R. T., Boyd, R. N., and Bhattacharjee, S. K., Organic Chemistry, 7th edition, Pearson
Prentice Hall, **2011**.
2. Pine, S. H., Organic Chemistry, Tata McGraw Hill, 5th edition, **2008**.
3. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith, Jerry March John Wiley & Sons, 6th edition, **2007**.
4. Finar, I. L., Organic Chemistry, Vol. 1 & 2, 5th edition, Longman Ltd., New Delhi, **1975**.
5. Guidebook to Mechanism in Organic Chemistry (6th Edition), Peter Sykes, Longman Scientific & Technical, **1985**.
6. Mukherjee, S.M., and Singh, S.P., Reaction Mechanism in Organic Chemistry, 1st edition, Macmillan India Ltd., New Delhi, **1990**.
7. Lowry, T. H., and Richardson, K. S., Mechanism and Theory in Organic Chemistry, 3rd edition, Addison – Wesley Longman Inc., **1998**.

Semester: 2 **Subject Code: CH0203** **Credits: 4** **4-0-0-4**

Title: Quantum Chemistry and Molecular Spectroscopy

Specific objectives:

To introduce advanced concepts in quantum chemistry, molecular spectroscopy and photochemistry.

Learning outcomes:

Ensures the students to understand, acquire knowledge on advanced concepts in quantum chemistry, molecular spectroscopy and photochemistry

Pre-requisite:

Basic mathematics and fundamentals of introductory quantum chemistry

Syllabus:

Quantum Chemistry II: Rigid rotor, energy levels of a rigid rotor, spherical harmonics, Schrödinger equation for the hydrogen atom – solutions, s orbitals, p orbitals, energy levels of a hydrogen atom in magnetic field, Schrödinger equation for Helium atom. Perturbation theory, Variational methods, Hartree-Fock equations, Self-consistent field methods for solving Hartree-Fock equations, Born-Oppenheimer approximation-molecular Hamiltonian operators, Valence bond treatment for chemical bonding in molecules, molecular orbitals, molecular orbital theory for different diatomic molecular systems, photoelectron spectra, SCF-LCAO-MO wave functions, electronic states of diatomic molecules, sp, sp^2 and sp^3 hybrid orbitals, molecular term symbols, Hückel molecular orbitals, bonding in polyatomic molecules.

Molecular spectroscopy: Characterization of electromagnetic radiation, energy quantization, atomic and molecular spectra, emission and absorption spectra; Fourier transformed spectroscopy, Lasers. Microwave spectroscopy, rotation spectra of di – and poly- atomic molecules; Stark effect; Applications of microwave spectra**.** Vibrational spectra of diatomic molecules; Rotation-vibration spectra of diatomic molecules; Vibrational spectra of diatomic and ploy atomic molecules; breakdown of Born-Oppenheimer approximation. Electronic spectra of diatomic and polyatomic molecules.

Photochemistry: Basics of Photochemistry and Photophysics, Jablonski diagram. Electronically excited states: electronic, vibrational and spin levels, unimolecular and bimolecular photophysical processes. Photochemical reactions and kinetics – energy transfer, electron transfer, excited state quenching – eximer and exiplex.

Prescribed Books

1. McQuarie, D.; Quantum chemistry, University Science Publishers, **2007.**
2. McQuarrie, D. A.; Simon, J. D.; Physical Chemistry: A Molecular Approach, University Science Books, **2011.**
3. Prasad, R. K.; Quantum Chemistry, New Age International Publishers, 4th edition, **2010.**
4. Banwell, C. N.; McCash, E. M.; Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill, 4th edition, **2010**.
5. Rohatgi Mukherjee K K , Fundamentals of Photochemistry, Wiley Eastern Ltd., **1992**.

Reference Books

1. Raff, L. M.; *Principles of Physical Chemistry*, Prentice Hall, **2001.**
2. Atkins, P. W.; Paula, J.; *Physical Chemistry*, Oxford Publications, 8th edition, **2009**.
3. Levine, I. N.; *Physical Chemistry*, McGraw-Hill Science/Engineering/Math, 6th edition, **2008.**
4. Kreyszig, Advanced Engineering Mathematics, 9th edition, **2012**.
5. Harris, D. C.; Bertolucci, M. D.; *Symmetry and Spectroscopy*: An Introduction to Vibrational and Electronic Spectroscopy, Dover Publications, **1989.**
6. Turro T J, Ramamurthy V, Scaiano J C, *Principle of molecular photochemistry* – An Introduction, University Science books, 1st edition, **2008**.

Semester: 2 **Subject Code: CH0204** **Credits: 4** **4-0-0-4**

Title: Physical methods in chemistry

Specific objectives:

To introduce spectroscopic techniques to solve structure of compounds.

Learning outcomes:

Ensures the students to understand, acquire knowledge on advanced concepts in spectroscopy thereby able to solve spectrum to structure.

Pre-requisite:

Basic spectroscopy and analytical chemistry

Syllabus:

Infra-Red Spectroscopy: Principle, instrumentation and sampling techniques, types of stretching and bending vibration – Factors influencing the vibrational frequency, vibrational frequencies of alkane, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenol, carbonyl compounds, amines and heterocyclics– related problems.

NMR Spectroscopy: ^{1}H NMR, Spectral parameters – intensity, chemical shift, multiplicity, coupling constant, factors affecting chemical shift. Analysis of first order and second - order spectra – shift reagents - structure determination of organic compounds by ^{1}H NMR spectra. Chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (^{1}H,^{13}C) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei (^{10}B) on the ^{1}H NMR spectra, Satellite spectra - examples for different spin systems – Systems with chemical exchange - study of fluxional behavior of molecules.

^{13}C NMR: Proton coupled; off–resonance decoupled; proton noise decoupled ^{13}C NMR spectra. Assignment of chemical shifts, additively effect, characteristic chemical shifts of common organic compounds and functional groups, APT, DEPT and INEPT spectra. NMR of common heteroatoms present in organic compounds - 2D NMR techniques ^{1}H – ^{1}H COSY, ^{1}H – ^{13}C COSY – HMBC, NOESY and INADEQUATE.

Elementary idea about mass spectrometry, interpretation of data and solving problems with spectroscopic techniques.

EPR spectroscopy and Magnetic Properties

Theory of EPR spectroscopy - Spin densities and McConnell relationship – Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy – Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes.

Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions.

Magnetic properties -Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature independent paramagnetism. Magnetic properties of lanthanides and actinides. Spin crossover in coordination compounds – Single molecule magnets.

Elementary idea about Mössbauer spectroscopy and NQR spectroscopy.

Prescribed books

1. Silverstein, R. M., and Webster, F. X., Spectrometric identification of organic compounds, John Wiley and Sons. Inc., 6th edition, **1997**.
2. W. Kemp, Organic Spectroscopy, 3rd edition, MacMillon, **1994**.
3. Jag Mohan, Organic Spectroscopy: Principles & Applications, Narosa Publishers, **2012**.
4. Drago, R. S., *Physical Methods for Chemistry*, 2nd Edition, Saunders College Publishing, **1992**.
5. Lever, A. B. P., *Inorganic Electronic Spectroscopy*, 2nd Sub. Edition, Elsevier Science, **1986**.

Reference Books

1. Pavia, Lampman and Kriz, Introduction to Spectroscopy, Brooks/Cole Pubs Co, 5th edition, **2015**.
2. Williams, D. H., and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, **1998**.
3. William Kemp, NMR in chemistry: A multinuclear introduction, MacMillan, **1988**.
4. Organic Spectroscopy by L. D. S. Yadav, Kulwer academic publishers, **2004**.
5. Gerson, F., and Huber, W., Electron Spin Resonance Spectroscopy for Organic Radicals, Wiley-VCH, 1st edition, **2001**.
6. Cotton, F. A., and Wilkinson, G., *Advanced Inorganic Chemistry*, 3rd edition, Wiley-Eastern Company, New Delhi, **1990**.
7. J. AND Wilkins Lewis, R. G., *Modern Coordination Chemistry Principles and Methods*, Interscience Publishers, Inc., **1967**.
8. Ebsworth, E. A. V., Structural Methods in Inorganic Chemistry, 3rd edition, ELBS, Great Britain, **1987**.
9. Scott, R. A., and Lukehart, C. M., Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, John and Wiley & Sons, LTD, **2007**.
10. Solomon, E. I., Lever, A. B. P., Inorganic Electronic Structure and Spectroscopy, Vol., 2, Applications and Case Studies, Wiley-Interscience, **2006**.
11. Satyanarayana, D. N., Electronic Absorption Spectroscopy, Universities Press, **2000**.
12. Jordon, R. B., Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd edition, Oxford University Press, **2007**.
13. Ballhausen, C. J., and Gray, H. B., Molecular Orbital Theory, Benjamin/Cummings Pub. Co, **1965**.
14. Figgis, B. N., and Hitchman, M. A., *Ligand Field Theory and Its Applications*, 1st edition, Wiley VCH, **1999**.

15. Huheey, J. E., Keiter, E. A. and Keiter, R. L., and Medhi, O. K., *Inorganic Chemistry - Principles of Structure and Reactivity*,4th Edition, Pearson Education, **2006**.
16. Purcell, K. F. and Kotz, J. C., *Inorganic Chemistry*, Cengage Learning, **2012**.

Semester: 2 Subject Code: CH0205 Credits: 3 0-1-5-3

Title: Advanced Physical Chemistry Laboratory I

Specific objectives:

To introduce experiments in thermochemistry, chemical kinetics, macromolecules, surface chemistry, photochemistry and electrochemistry.

Learning outcomes:

The students will obtain hands on experience on the instrumentation and experimental techniques to measure physico-chemical parameters such as thermodynamic, electrochemical, kinetics and equilibrium parameters. Also, will get experience in the analysis and the interpretation of data.

Pre-requisite:

Undergraduate level physical chemistry concepts. Advanced experiments on thermodynamics, kinetics, catalysis, electrochemistry, spectroscopy characterization methods and macromolecules.

Syllabus:

Advanced experiments on thermodynamics, kinetics, catalysis, electrochemistry, spectroscopy, photochemistry and macromolecules.

Reference Books

1. In-house laboratory manual, Department of Chemistry, CUTN.
2. Halpern, A. M.; McBane, G. C. *Experimental Physical Chemistry*: A Laboratory Prescribed Book, 3rd ed.; W. H. Freeman, 2006.

Semester: 3 **Subject Code: CH0301** **Credits: 4** **4-0-0-4**

Title: Bio-Inorganic Chemistry and Inner Transition Elements

Specific objectives:
To introduce the principles of bioinorganic chemistry and advanced nuclear chemistry and the chemistry of f-block elements.

Learning outcomes:

Ensures the students to understand, concepts concepts of Bioinorganic Chemistry, Function and Transport of Alkali and Alkaline earth metals, Metalloporphyrins / Metalloenzymes, Nuclear Chemistry and Inner Transition elements

Pre-requisite:

Inorganic Chemistry & Coordination Chemistry

Syllabus:

General Principles of Bioinorganic Chemistry: Occurrence and availability of Inorganic elements in biological systems. Basics of Bio mineralisation.

Function and Transport of Alkali and Alkaline earth metals: Uptake, transport and storage of metal ions by organisms - structure and functions of biological membranes - the generation of concentration gradients (the Na^+ -K^+ pump) - mechanisms of ion-transport across cell membranes – bleomycin - siderophores (e.g. enterobactin and desferrioxamine) - transport of iron by transferring - storage of iron by ferritin - bio chemistry of calcium as hormonal messenger. Metals at the Center of Photosynthesis: Primary Processes in Photosynthesis – Photosystems I and II.

Metalloporphyrins/Metalloenzymes: Dioxygen transport and storage - hemoglobin and myoglobin: electronic and spatial structures - hemeythrin and hemocyanine - synthetic oxygen carriers, model systems - blue copper proteins (Cu) - iron-sulfur proteins (Fe)-cytrochromes electron transport chain - carbon monoxide poisoning - iron enzymes - peroxidase, catalase and cytochrome P-450, copper enzymes - superoxide dismutase, carboxypeptidase, carbonicanhydrase, vitamin B_{12} and B_{12} coenzymes, nitrogen fixation.

Medicinal bioinorganic chemistry: platinum complexes in cancer therapy – cis-platin and its mode of action – metal toxicity.

Advanced Nuclear Chemistry: Radiochemical principles in the use of tracers - applications of radioisotopes as tracers - chemical investigations, analytical applications, agricultural and industrial applications - neutron activation analysis - carbon and rock dating - use of nuclear reactions - radioisotopes as source of electricity - nuclear medicines. Radiolysis of water and hydrated electron.

Inner Transition elements: Special features of f-block elements, introduction, occurrence, separation, oxidation states, lanthanide contraction, coordination number, structures, and simple reactions. Spectral, Magnetic properties and Analytical applications.

Prescribed Books

1. Lippard, S. J., and Berg, J. M., *Principles of Bioinorganic Chemistry*, Panima Publishing Company, New Delhi, **1997**.
2. Kaim W., and Schewederski, B., *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, John Wiley & Sons, New York, USA, **2013**.
3. Bertini, I., Gray, H. B., Lippard, S. J. and Valentine, J. S., *Bioinorganic Chemistry*, 1st South Asia edition, Viva books Pvt. Ltd., **2007**.
4. Huheey, J. E., Keiter, E. A. and Keiter, R. L., and Medhi, O. K., *Inorganic Chemistry - Principles of Structure and Reactivity*,4th edition, Pearson Education, **2006**.
5. Behrens, P., Bauerlein, E., *Hand Book of Biomineralization*, 1st edition, Vol. 1& 2, Wiley-VCH, **2007**.
6. Arnikar, H. J., Essentials of Nuclear Chemistry, 4th edition, New Age International Publishers Ltd., New Delhi, **1995**.
7. Loveland, W. D., Morrissey, D. J., Seaborg, G. T., *Modern Nuclear Chemistry*, Wiley-VCH Verlag GmbH Co. KGaA, **2006**.
8. Glasstone,'*Source Book on Atomic Energy'*, 3rd edition, Affiliated East West Press, **1979.**
9. Lee, J. D. *Concise Inorganic Chemistry*, Blackwell Science, 5th edition, **1996.**

Reference Books

1. Purcell, K. F. and Kotz, J. C., Inorganic Chemistry, Cengage Learning, **2012**.
2. Cotton, F. A., Wilkinson, G., Carlos A. Murillo, Manfred Bochmann, Advanced Inorganic Chemistry, 6th ed., A Wiley - Interscience Publication, John –Wiley & Sons, USA, **2007**. Chem. Education, 62, No. 11, Bioinorganic Chemistry, State of the Art. **1985.**
2. Eichorn, G. L., Inorganic Biochemistry, Volumes 1 & 2, 2nd ed., Elsevier Scientific Publishing Company, New York, **1973**.
3. Atkins, P., Overton, T., Rourke, J., Weller M., and Armstrong, F., Inorganic Chemistry, 5th edition, Oxford University Press, **2010.**
4. Lehninger, A., Nelson, D. L., Cox, M. M, Principles of Biochemistry, 5th edition, W.H Freeman, **2008.**
5. Alessio, E., Bioinorganic Medicinal Chemistry, 1st Edition, Wiley-VCH Verlag GmbH Co. KGaA, **2012**.

Semester: 3 **Subject Code: CH0302** **Credits: 4** **4-0-0-4**

Title: Advanced organic synthesis

Specific objectives:

To introduce retrosynthetic analysis and modern synthetic reagents

Learning outcomes:

The students will acquire knowledge on disconnection approach as well as role of modern synthetic reagents in organic transformations

Pre-requisite:

Organic reaction mechanism.

Syllabus:

Oxidations and reductions: oxidation: Ozone, CrO_3, DCC, DDQ, 9-BBN, lead tetra acetate, phenyl iodoso acetate, dimethyl sulphoxide, SeO_2, PCC, and Yeast in organic synthesis and functional group transformations. Phase transfer catalysis – benzyltriethylammonium halides- crown ethers. Reduction**:** Addition of hydrogen at carbon-carbon multiple bonds – catalytic hydrogenation of carbonyl and other functional groups – group-III hydride-donor reagents – group-IV hydride donors – reduction reactions involving hydrogen atom donors – dissolving-metal reductions – reductive deoxygenation of carbonyl groups – reductive elimination and fragmentation.

Organometallic reagents: B, Mg, Li, Si, Pd, Cu, Zn, Ru, Rd, Sm, In, Sn, Cd, Hg, Ce, homogeneous hydrogenation - Willkinson's catalyst – umploung synthesis.

Protection and deprotection of organic functional groups – alcohol, amines and carbonyl compounds.

Planning Organic Synthesis: An introduction to reterosynthesis - synthon – synthetic equivalent – target molecule, functional group interconversion. Disconnection approach- one group disconnection- disconnection of alcohols, olefins and ketones.Logical and illogical disconnections. Two group disconnection-1, 2, -1, 3, 1, 4, 1, 5 and -1, 6 dioxygenated skeletons and dicarbonyls. Green chemical synthesis.

Recommended Books:

1. Carey F. A., and Sundberg, R. A., Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5th edition, Springer, New York, **2007**.
2. Carruthers, W., and Coldham, I., Modern methods of Organic Synthesis, 1st South Asian

Edition, Cambridge University Press, **2005**.
3. March, J., and Smith, M. B., March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure 6th edition, Wiley, **2007**.
4. Warren, S., Wyatt, P., Organic Synthesis: The Disconnection Approach, Wiley, **2008**.
5. Willis, C. L., Wills, M., Organic Synthesis, Oxford Chemistry Primers, 31, Oxford Science
Publications, **1996**.
6. Paquette, L. A., Crich , D., Fuchs, P. L., Molander, G. A., Encyclopedia of Reagents for Organic Synthesis, 14 Volume Set, Wiley, **2009**.
7. Warren, S., Wyatt, P., Wiley, Workbook for Organic Synthesis: The Disconnection Approach, 2nd edition, **2010**.
8. Starkey, L., S., Introduction to Strategies for Organic Synthesis, Wiley, **2012**.
9. Anastas, P. T., Green Chemistry: Theory and Practice, Oxford University Press, USA, **2000**.

Semester: 3 **Subject Code: CH0303** **Credits: 4** **4-0-0-4**

Title: Statistical Thermodynamics, Chemical Kinetics and Electrochemistry

Specific objectives:

To introduce statistical thermodynamics, chemical kinetics and electrochemistry.

Learning outcomes:

The students will acquire knowledge on statistical thermodynamics, advanced chemical kinetics, surface analytical techniques to measure surface properties of materials and the advanced principles of various electrochemical techniques.

Pre-requisite:

Basic thermodynamics, chemical kinetics and electrochemistry.

Syllabus:

Statistical Thermodynamics: Statistical entropy, microcanonical and canonical ensembles, Maxwell-Boltzmann distribution, Thermodynamic quantities and canonical partition function, molecular partition functions, translational, rotational, vibrational and electronic partition functions. Ideal monoatomic and diatomic gases. Heat capacities - Einstein theory and Debye theory. Applications of statistical thermodynamics to activated complex theory.

Chemical Kinetics: Enzyme kinetics – Michaelis-Menten kinetics, Multi-substrate reactions, Lineweaver-Burk plot; Kinetics of fast and complex reactions: flow and relaxation methods; ultrafast reactions.

Solids, Surface growth and characterization: Growth and structure of solid surfaces, surface analytical techniques (XPS, Auger) and characterization. Solid solutions, solubility limit, phase rule, binary phase diagrams, intermediate phases, intermetallic compounds, Alloys.

Principles of electrochemistry and techniques: Theory of strong electrolytes; electrified interfaces: theories and models; basics in electro-catalysis and bio-electrochemistry; kinetics of electrode reactions; irreversible electrode processes. Cyclic voltammetry, differential pulse voltametry and square wave voltammetry, polarography, amperometry.

Prescribed Books

1. McQuarrie, D. A.; Simon, J. D.; Physical Chemistry: A Molecular Approach, University Science Books, **2011.**
2. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.
3. McQuarrie, D. A.; Statistical mechanics, University Science Publishers, **2000.**
4. J.O'M Bockris and A.K.N Reddy, Modern Electrochemistry 2A: Fundamentals of Electrodics, Vol II, **2001**.
5. D. Skoog and D.West , Principles of Instrumental Analysis, Cengage Learning; 6th edition, **2006**

Reference Books

1. Hill, T. A.; an Introduction to Statistical Thermodynamics, Dover Publications Inc., **1987**.
2. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6th edition, **2008**.
3. Laidler, K. J.; Chemical Kinetics, Pearson Education, 3rd edition, **2011**.
4. D.R. Crow, Principles and Applications of Electrochemistry, John Wiley & Sons (New York) 2nd edition, **2001.**
5. Bard, A. J.; Faulkner, L. R.; Electrochemical Methods: Fundamentals and Applications, Wiley, 2nd edition, **2000.**

Semester: 3 **Subject Code: CH0304** **Credits: 3** **0-0-3-3**

Title: Advanced Inorganic Chemistry Laboratory I

Specific objectives:

To introduce multistep inorganic compound synthesis and its spectroscopic analysis, separation and estimation of organic compounds.

Learning outcomes:

Ensures the students to understand, acquire knowledge and have hands on experience in multistep inorganic compound synthesis and analysis by using spectroscopic techniques. Separation techniques.

Pre-requisite:

Single step preparations and course

Syllabus:

A. Estimation of metal ions using spectrophotometry
B. Synthesis, separation, purification of inorganic compounds and characterization by using various spectroscopic and analytical techniques

Reference Books

1. Elias, A. J., *A Collection of Interesting General Chemistry Experiments*, Universities Press, Sangam Books Ltd, **2002**.
2. Woollins, J. D., *Inorganic experiments*, 3rd edition, Wiley-VCH Verlag GmbH @Co. KGaA, **2012**.
3. Hein, M., Peisen, J. N., and Miner, R. L., *Foundations of College Chemistry in the Laboratory*, John Wiley and Sons, **2011**.
4. Girolami, G. S., Rauchfuss,T. B., and Angelici, R. J., Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, 3rd edition, University Science Books, **1999**.
5. Jolly, W. L., The Synthesis and Characterization of Inorganic Compounds, Prentice-Hall, Inc.**1970**.
6. In-house Laboratory Manual, Department of Chemistry, CUTN.

Semester: 4 **Subject Code: CH0401** **Credits: 6** **0-2-12-6**

Title: Research Project

Research project is carried out under the supervision of a teacher in the chosen field by the student. Normally it will be continuation of literature survey carried out from the yester semester.

List of Electives (Semester I to IV)

Course Code	Title of the Course	Credits
CYE001	Principles of Polymer Science	3
CYE002	Principles of Fluorescence Spectroscopy	3
CYE003	Asymmetric Catalysis	3
CYE004	Essentials of Carbohydrate Chemistry	3
CYE005	Organic Electronics	3
CYE006	Photochemistry in Molecules and Materials	3
CYE007	Medicinal Inorganic Chemistry	3
CYE008	Organic Semiconductors	3
CYE009	Advances in Polymer Science	3
CYE010	Advances in Carbohydrate Research	3
CYE011	Advanced Organic Materials and Catalysis	3
CYE012	Chemistry of CH Activation	3
CYE013	Advanced Bio-inorganic Chemistry	3
CYE014	Principles of Biochemistry	3
CYE015	Mathematics for Chemists and biologists	3
CYE016	Fundamentals of Analytical Chemistry	3
CYE017	Electrochemical Energy Systems	3