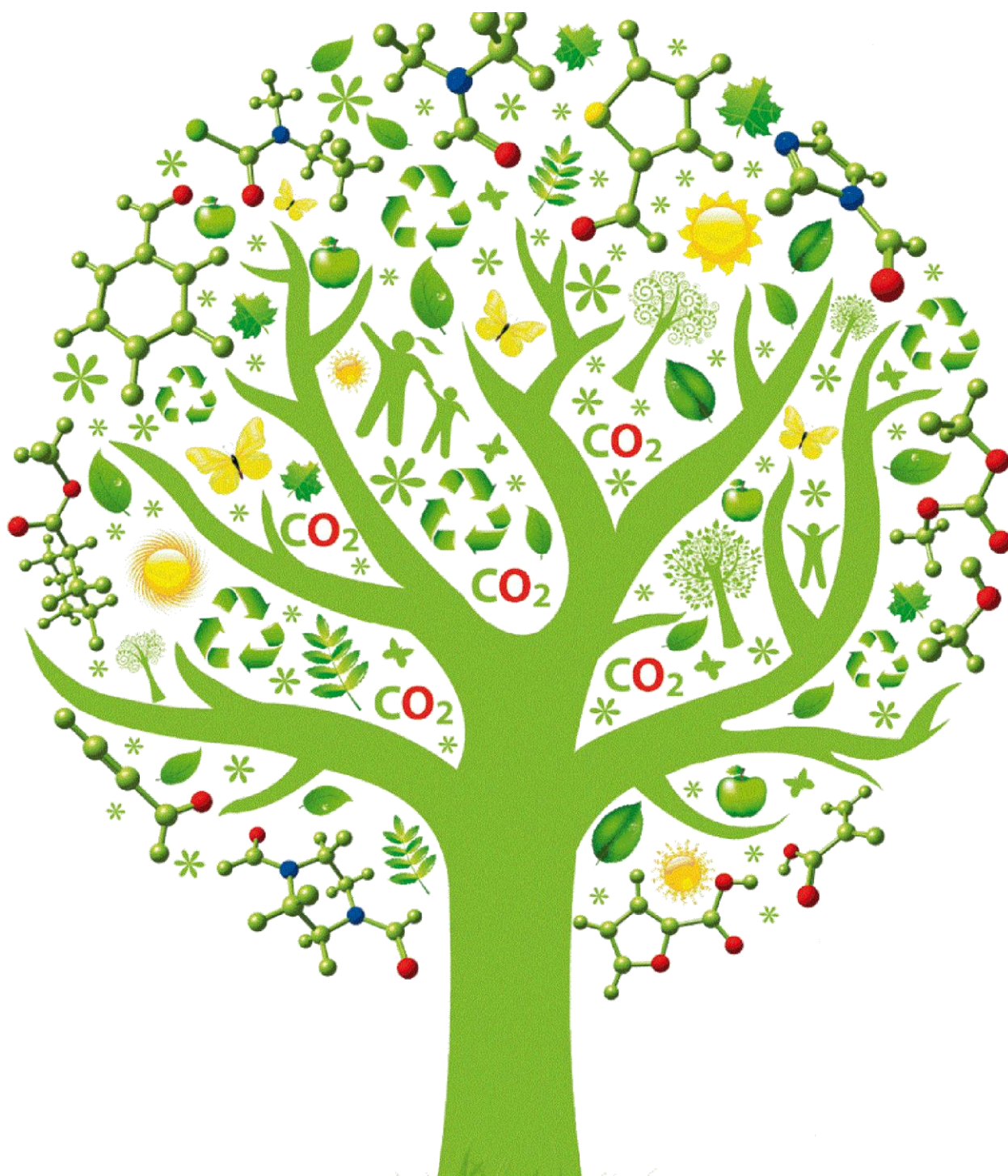


# M.Sc Chemistry



**Department of Chemistry**

**Central University of Tamil Nadu**

**Thiruvarur 610 101**

Name of the course	:	<b>M. Sc. (Chemistry)</b>
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 of age as on 01-07-2015.

## Contents and Credits

Course Code	Title of the Course	Credits
CY4101	Advanced Inorganic Chemistry I	4
CY4102	Advanced Organic Chemistry I	4
CY4103	Advanced Physical Chemistry I	4
CY4104	Advanced Physical Chemistry Laboratory I	3
CY****	ELECTIVE	3
CY4201	Advanced Inorganic Chemistry II	4
CY4202	Advanced Organic Chemistry II	4
CY4203	Advanced Physical Chemistry II	4
CY4204	Physical methods in Chemistry	4
CY4210	Advanced Organic Chemistry Laboratory I	3
CY****	ELECTIVE	3
CY5101	Advanced Inorganic Chemistry III	4
CY5102	Advanced Organic Chemistry III	4
CY5103	Advanced Physical Chemistry III	4
CY5104	Seminar and Literature Review	3
CY5110	Advanced Inorganic Chemistry Laboratory I	3
CY****	ELECTIVE	3
CY5201	Research Project	9
CY****	ELECTIVE	3
		73

Semester: 1

Subject Code: CY4101

Credits: 4

4-0-0-4

**Title: Advanced Inorganic chemistry I**

**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<sub>2</sub> type crystal structures – layer structures - lattice energy - Born-Landé, 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 – Spectral and magnetic properties of complexes – 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. Spectral and magnetic properties of lanthanides and actinides.

**Prescribed Books**

1. Huheey J. E., Keiter E. A. and Keiter R. L. and Medhi O. K., *Inorganic Chemistry - Principles of Structure and Reactivity*, 4<sup>th</sup> edition, Pearson Education, **2006**.
2. Atkins, P. W.; Paula, J.; *Physical Chemistry*, Oxford Publications, 8<sup>th</sup> edition, **2009**.
3. B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3<sup>rd</sup> edition, John Wiley & Sons, **2010**.
4. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, 3<sup>rd</sup> 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. 2<sup>nd</sup> 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*, 3<sup>rd</sup> edition, Pearson, **2004**.
5. Housecraft, C. E., and Alan G. Sharpe, *Inorganic Chemistry*, 4<sup>th</sup> 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. Wulfborg, G., *Inorganic Chemistry*, University Science Books, **2000**.

Semester: 1

Subject Code: CY4102

Credits: 4

4-0-0-4

### Title: Advanced Organic Chemistry I

**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*, 4<sup>th</sup> 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*, 5<sup>th</sup> edition, **2007**.
4. *Heterocyclic Chemistry-* J. A. Joule, K. Mills, G. F. Smith, Blackwell publishing Ltd, 5<sup>th</sup> 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: CY4103**

**Credits: 4**

**4-0-0-4**

**Title: Advanced Physical Chemistry I**

**Quantum Chemistry I:** Wave particle duality and uncertainty principle, 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 C<sub>2v</sub>, C<sub>3v</sub> and D<sub>2h</sub>, 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., 3<sup>rd</sup> edition, **2009**.
2. Veera Reddy, K., Symmetry and spectroscopy of molecules, New Age International, 2<sup>nd</sup> 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, 8<sup>th</sup> edition, **2009**.
3. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6<sup>th</sup> 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: CY4104

Credits: 3

0-1-5-3

**Physical Chemistry Laboratory**

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

**Reference Books**

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

Semester: 1

Subject Code: CYxxxx

Credits: 3

3-0-0-3

Mathematics for Chemists (CY0001) or Biology for Chemists (CY0002)

Semester: 8

Subject Code: CY4201

Credits: 4

4-0-0-4

**Title: Advanced Inorganic Chemistry II**

**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.  $\sigma$ -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 – Evaluation of  $10Dq$  and  $\beta$  for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra – electronic spectra of  $[\text{Ru}(\text{bipy})_3]^{2+}$ . Optical rotatory dispersion, circular dichroism and Magnetic circular dichroism – applications to metal complexes.

**Infrared and Raman Spectroscopy:** Vibrations in simple molecules ( $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ) 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*, 2<sup>nd</sup> 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*, 4<sup>th</sup> 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*, 2<sup>nd</sup> edition, Saunders College Publishing, **1992**.
8. Lever, A. B. P., *Inorganic Electronic Spectroscopy*, 2<sup>nd</sup> Sub. edition, Elsevier Science, **1986**.

### Reference Books

1. Elschenbroich, C., and Salzer, A., *Organometallics: A Concise Introduction*, 3<sup>rd</sup> edition, **1999**.
2. Greenwood, N. N., and Earnshaw, A., *Chemistry of the Elements*, 2<sup>nd</sup> edition, Elsevier, **2005**.
3. Jolly, W. L., *Modern Inorganic Chemistry*, McGraw Hill, New York, 2<sup>nd</sup> Edition., **1991**.
4. Douglas, B., McDaniel, D., and Alexander, J., *Concepts and Models of Inorganic Chemistry*, John Wiley, New York, 3<sup>rd</sup> edition., **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*, 2<sup>nd</sup> 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., Norton, J. R. and Finke, R. G., *Principles and Applications of Organotransition Metal Chemistry*, University Science Books. Mill Valley, California, **1987**.

Semester: 8

Subject Code: CY4202

Credits: 4

4-0-0-4

### Title: Advanced Organic Chemistry II

**Pericyclic Reactions:** Pericyclic reactions – orbital correlation diagram – FMO. Diels-Alder reactions – 1,3-dipolar cycloaddition reactions – [2+2] cycloadditions and related reactions leading to cyclobutanes – [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.

**Application of molecular Rearrangements in organic synthesis:** 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 rearrangements.

**Selected name reactions in organic synthesis:** Wittig Reaction, Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakura reaction, Tishcheko reaction and Ugi reaction.

**Prescribed books**

1. Carey F.A., and Sundberg, R.J., Advanced Organic Chemistry, Part B: Reactions and synthesis, 5<sup>th</sup> 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**.

**Reference books**

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

**Semester: 8****Subject Code: CY4203****Credits: 4****4-0-0-4****Title: Advanced Physical Chemistry II**

**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<sup>2</sup> and sp<sup>3</sup> 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 poly 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. McQuarrie, 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, 4<sup>th</sup> edition, **2010**.
4. Banwell, C. N.; McCash, E. M.; Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill, 4<sup>th</sup> 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, 8<sup>th</sup> edition, **2009**.
3. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6<sup>th</sup> edition, **2008**.
4. Kreyszig, Advanced Engineering Mathematics, 9<sup>th</sup> 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, 1<sup>st</sup> edition, **2008**.

**Semester: 8****Subject Code: CY4204****Credits: 4****4-0-0-4****Title: Physical methods in chemistry**

**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:** <sup>1</sup>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 <sup>1</sup>H NMR spectra. Chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (<sup>1</sup>H,<sup>13</sup>C) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei (<sup>10</sup>B) on the <sup>1</sup>H NMR spectra, Satellite spectra - examples for different spin systems – Systems with chemical exchange - study of fluxional behavior of molecules.

<sup>13</sup>C NMR: Proton coupled; off–resonance decoupled; proton noise decoupled <sup>13</sup>C NMR spectra. Assignment of chemical shifts, additivity 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 <sup>1</sup>H – <sup>1</sup>H COSY, <sup>1</sup>H – <sup>13</sup>C COSY – HNBC, 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., 6<sup>th</sup> edition, **1997**.
2. W. Kemp, Organic Spectroscopy, 3<sup>rd</sup> edition, MacMillan, **1994**.
3. Jag Mohan, Organic Spectroscopy: Principles & Applications, Narosa Publishers, **2012**.
4. Drago, R. S., *Physical Methods for Chemistry*, 2<sup>nd</sup> 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, 5<sup>th</sup> 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*, 3<sup>rd</sup> 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, 3<sup>rd</sup> 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*, 1<sup>st</sup> 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*, 4<sup>th</sup> Edition, Pearson Education, **2006**.
16. Purcell, K. F. and Kotz, J. C., *Inorganic Chemistry*, Cengage Learning, **2012**.

Semester: 2

Subject Code: CY4210

Credits: 3

0-1-5-3

**Title: Advanced Organic Chemistry Laboratory I**

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,  $^1\text{H}$  and  $^{13}\text{C}$  NMR techniques.

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

Quantitate Analysis: Estimation of common organic compounds

**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, 5<sup>th</sup> edition, Pearson education Ltd, **1996**.

**Reference Books:**

1. Leonard, J., Lygo, B., Procter, G., Advanced Practical Organic Chemistry, , 3<sup>rd</sup> 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., 6<sup>th</sup> edition, **1997**.

Semester: 2

Subject Code: CYXXXX

Credits: 3

3-0-0-3

Semester: 3

Subject Code: CY5101

Credits: 4

4-0-0-4

**Title: Advanced Inorganic Chemistry III**

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

**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  $\text{Na}^+$ - $\text{K}^+$  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 - biochemistry 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 - heme-thyrin and hemocyanine - synthetic oxygen carriers, model systems -

blue copper proteins (Cu) - iron-sulfur proteins (Fe)- cytochromes electron transport chain - carbon monoxide poisoning - iron enzymes - peroxidase, catalase and cytochrome P-450, copper enzymes - superoxide dismutase, vitamin B<sub>12</sub> and B<sub>12</sub> coenzymes, nitrogen fixation. Medicinal bioinorganic chemistry: platinum complexes in cancer therapy – cis-platin and its mode of action.

**Advanced Nuclear Chemistry:** Radioactive equilibrium: Transient and secular -nuclear reactions: energetics and types - nuclear fission- liquid drop model-shell model - nuclear spin calculation -Nordheim's rule - nuclear fusion - essential features of nuclear reactors - application of radioisotopes: Probing by isotopes, reactions involved in the preparation of radioisotopes, the Szilard-Chalmer's reaction - 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.

### 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*, 1<sup>st</sup> 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*, 4<sup>th</sup> edition, Pearson Education, **2006**.
5. Behrens, P., Bauerlein, E., *Hand Book of Biomineralization*, 1<sup>st</sup> 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', 3<sup>rd</sup> edition, Affiliated East West Press, **1979**.

### 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: CY5102

Credits: 4

4-0-0-4

### Title: Advanced Organic Chemistry III

**Oxidations and reductions:** oxidation: Ozone, CrO<sub>3</sub>, DCC, DDQ, 9-BBN, lead tetra acetate, phenyl iodoso acetate, dimethyl sulphoxide, SeO<sub>2</sub>, PCC, 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, Rh, Sm, In, Sn, Cd, Hg, Ce, homogeneous hydrogenation - Willkinson's catalyst – umpolung synthesis.

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

**Planning Organic Synthesis:** An introduction to retrosynthesis - 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, 5<sup>th</sup> edition, Springer, New York, **2007**.
2. Carruthers, W., and Coldham, I., Modern methods of Organic Synthesis, 1<sup>st</sup> 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, 2<sup>nd</sup> 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: CY5103**

**Credits: 4**

**4-0-0-4**

**Title: Advanced Physical Chemistry III**

**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:** Theories of unimolecular gaseous reactions: Lindmann, Lindmann-Hinselwood, RRK, RRKM theories. Kinetics of fast reactions: flow and relaxation methods; ultrafast reactions.

**Solids, Surface growth and characterization:** Growth and structure of solid surfaces, surface analytical techniques 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 voltammetry 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, 8<sup>th</sup> 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 Electroics, Vol II, **2001**.
5. D. Skoog and D. West, Principles of Instrumental Analysis, Cengage Learning; 6<sup>th</sup> 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, 6<sup>th</sup> edition, **2008**.
3. Laidler, K. J.; Chemical Kinetics, Pearson Education, 3<sup>rd</sup> edition, **2011**.
4. D.R. Crow, Principles and Applications of Electrochemistry, John Wiley & Sons (New York) 2<sup>nd</sup> edition, **2001**.
5. Bard, A. J.; Faulkner, L. R.; Electrochemical Methods: Fundamentals and Applications, Wiley, 2<sup>nd</sup> edition, **2000**.

**Semester: 3**

**Subject Code: CY5104**

**Credits: 3**

**0-0-3-3**

#### **Title: Seminar and Literature Review**

Students are required to take two seminars of one hour duration. 45 minutes presentation and 15 minutes of questions and discussion. Evaluation will be based on content of the material, presentation and depth of knowledge in the topic presented.

The student will be required to make a literature survey for the project that will be carried out in the subsequent semester assigned to a teacher. There won't be any external written examination.

**Semester: 3**

**Subject Code: CY5110**

**Credits: 3**

**0-0-3-3**

#### **Title: Inorganic Chemistry Laboratory**

Estimation of copper, iron and nickel using spectrophotometry.

#### **Preparation of the following compounds and their Characterization**

- |  |                                      |
|--|--------------------------------------|
| 1. Tetramminecopper(II) sulphate.      | 5. Dibenzyltin dichloride.           |
| 2. Potassium trioxalatochromate(III).  | 6. Nitro and nitrito linkage isomers |
| 3. Potassium trioxalatoaluminate(III). | 7. Mn <sub>3</sub> clusters          |
| 4. Trithioureacopper(I) chloride.      |                                      |
1. Synthesis and study of Tris(oxalato)iron(III) potassium salt by Cyclic Voltammetry (CV) and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction

- potential ( $E^{\circ}$ ); the number of electrons transferred in the redox process ( $n$ ); the diffusion coefficient ( $D$ ); electrochemical reversibility; and the effects of varying concentration ( $C$ ) and scan rate.
- Synthesis and study of  $Mn^{III}(Salen)Cl$  by Cyclic Voltammetry and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential ( $E^{\circ}$ ); the number of electrons transferred in the redox process ( $n$ ); the diffusion coefficient ( $D$ ); electrochemical reversibility; and the effects of varying concentration ( $C$ ) and scan rate.
  - Preparation and determination of the effective magnetic moment and number of unpaired electrons in  $Mn(acac)_3$ .
  - Preparation and determination of the aquation rate of  $[Co(NH_3)_5Cl]Cl_2$ .
  - Preparation and resolution of the optically active compound  $[Co(en)_3]^{3+}$ .
  - Preparation and characterization of (Mesitylene) tricarbonylmolybdenum(0) by solution infrared spectrum.
  - Bioanalytical techniques – Monitoring the cleavage of DNA and protein by metal complexes using Gel electrophoresis techniques – Agarose and PAGE

### Reference Books

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

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

**Semester: 4                      Subject Code: CY5201                      Credits: 9                      0-3-12-9**

### 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.

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

### List of Electives

Mathematics for chemists and biologists, Introductory Biology, Advanced Spectroscopy Techniques, Principles of Fluorescence, Medicinal Inorganic Chemistry, Supramolecular Chemistry, Molecular Electronics, Chemistry of Soft matter, Carbon nanomaterials, Advances in Carbohydrate Chemistry, Fundamentals of Polymer Chemistry, Advances in Polymer Chemistry, Organophosphorus Chemistry and Applications, Chemistry of Biotransformations, Asymmetric Catalysis, Asymmetric Synthesis, Medicinal Chemistry and Drug design, Chemistry of C-H Activation, Chemistry of Materials, Imaging Techniques.

**Mathematics for Chemists and biologists**

**Subject Code: CY0001**

**Credits: 3**

**3-0-0-3**

Scalars and Vectors: Scalars, Vectors, Vector Products, Vector Spaces, linear independence, basis, curvilinear coordinates, Tensors. Applications: Two body problem, Center of Mass and Relative coordinates.

Vector Integration and Differentiation: Gradient, Divergence and Curl, Line Integrals, Surface integrals, volume integrals, Greens theorem, Stokes Theorem. Applications: Force, Work and Potentials. Path integrals.

Matrix Algebra: Matrices, Rank, Determinants, Eigenvalues, Eigenvectors, System of Equations. Applications: Slater Determinants, Huckel MO theory.

1st order ODEs: Differential Equations of 1st order. Separation of variables, integrating factor, exact differentials, system of ODEs. Applications: Reaction rates. 2nd order differential equations: 2nd order differential equations with constant coefficients, general solution, particular solution, power series method. Applications: Angular Momentum Eigen functions for a single particle.

Numerical Methods: Taylor series, numerical differentiation and integration, matrix diagonalization methods. Applications: Perturbation method for radiation-matter interaction

Reference books:

1. Kreyszig, Advanced Engineering Mathematics, 9<sup>th</sup> edition, **2012**.
2. Peter Tebbutt, Basic Mathematics for Chemists, 2nd Edition, Wiley, **1998**.

**Introductory Biology****Subject Code: CY0002****Credits: 3****3-0-0-3****Objectives :**

1. To enable the student to develop a sound knowledge of fundamental concepts in biology.
2. To enumerate the molecular motif of a living cell, structural and functional hierarchy of biomolecules.
3. To emphasis on the various aspects of metabolism and interrelationship of metabolic events.

**UNIT 1: Amino acids and Proteins**

**Living Cell** – Plant and Animal cell. Cell membrane – organelles – functions of major subcellular components.

**Amino acids** – Classification –Synthesis of  $\alpha$ -amino acids and their identification. Peptide bond-stereochemistry, synthesis of peptides.

**Proteins** – Classification – properties-3D structure-determination of amino acid sequence – denaturation and renaturation of protein molecules.

**UNIT 2 : Enzymes & lipids**

Nomenclature, classification and properties-specificity, factors influencing enzyme action. Mechanism of enzyme action – Lock and Key model and induced fit models. Coenzymes – cofactors – prosthetic groups of enzymes (TPP, NAD, NADP, FAD, ATP).

Classification and properties of lipids. Hydrolysis-acid number, saponification number. Metabolism: Oxidation of glycerol –  $\beta$ -oxidation of fatty acids; biosynthesis of lipids – synthesis of fatty acids and synthesis of triglycerides.

**UNIT 3: Carbohydrates**

Carbohydrates of the cell membrane – starch, cellulose and glycogen. (Structure and utility) Metabolism: Glycolysis and its reversal; TCA cycle. Relation between glycolysis and respiration. Principles of bioenergetics, electron transport chain and oxidative phosphorylation. Self study: Gluconeogenesis, pentose phosphate pathway.

**UNIT 4: Nucleic Acids**

Nucleosides and nucleotides – purine and pyrimidine bases. Nucleic acids Difference between DNA and RNA. Classification of RNA. Biosynthesis of DNA: Replication. Biosynthesis of mRNA: Transcription. Genetic code – mutations and mutants. DNA repair. Biosynthesis of proteins. DNA sequencing and PCR, recombinant DNA technology, DNA polymorphism.

**Text books**

1. David L. Nelson and Michael M. Cox Lehninger, Principles of Biochemistry, Fourth Edition, , Worth Publishers, New York, **2005**.
2. Lubert Stryer, Biochemistry, W. H. Freeman and company, New York, **1975**.
3. Robert L.Caret, Katherine J. Denniston, Joseph J. Topping, Principles and Applications of organic and biological chemistry, WBB publishers, USA, **1993**.
4. A. Mazur and B. Harrow, Text book of biochemistry, 10th Edition, W.B. Saunders Co., Philadelphia, **1971**.