

# **School of Applied Sciences**

# **Centurion University of Technology & Management**

M.Sc. (Applied Chemistry)

(Two years programme)

2017

#### M.Sc. Chemistry (Two year programme) Course Structure

	Course Structure							
Seme	Semester-I							
	Sl. No Code Subject Name		Subject Name	L-T-P	Credits			
	1	MSCC1101	Advanced Physical Chemistry I	4-1-0	4			
2 MSCC1102		MSCC1102	Advanced Inorganic Chemistry I	4-1-0	4			
3 MSCC1103		MSCC1103	Advanced Organic Chemistry I	4-1-0	4			
4 MSCC1104		MSCC1104	Polymer Chemistry	4-1-0	4			
5 MSCC1105		MSCC1105	Chemistry Laboratory 1	0-0-6	4			
6			Skill Elective I	0-0-6	4			
			Total		24			

## Semester-II

Sl. No	Code	Subject Name	L-T-P	Credits
1	MSCC1201	Advanced Physical Chemistry II	4-1-0	4
2	MSCC1202	Advanced Inorganic Chemistry II	4-1-0	4
3	MSCC1203	Advanced Organic Chemistry II	4-1-0	4
4	MSCC1204	Nuclear Chemistry	4-1-0	4
5	MSCC1205	Chemistry Laboratory 2	0-0-6	4
6		Skill Elective II	0-0-6	4
		Total		24

#### **Skill Elective - I**

Sl. No	Code	Subject Name	L-T-P	Credits
1	SBFE3127	Water Quality Analysis	0-0-3	4
2	MSCC1001	Pharmaceutical Chemistry	0-0-3	4

#### **Skill Elective - II**

Sl. No	Code	Subject Name	L-T-P	Credits
1	SBFE3152	Clinical Practice lab	0-0-3	4
2	MSCC1002	Analytical Chemistry	0-0-3	4

#### Semester-III

Sl. No	V		L-T-P	Credits
1	MSCC2301	Advanced Inorganic Chemistry III	4-1-0	4
2	MSCC2302	Advanced Organic Chemistry III	4-1-0	4
3	MSCC2303	Advanced Physical Chemistry III	4-1-0	4
4	MSCC2304	Advanced Solid State Chemistry	4-1-0	4
5	MSCC2305	Chemistry Laboratory 3	0-0-6	4
6	MSRM5101	Introduction To Research	0-0-2	2
7	MSCC2306	Green Chemistry Lab	0-0-3	2
		Total		24

## Semester-IV

Sl. No	Code	Subject Name	L-T-P	Credits
1	MSCC2401	MSCC2401 Advanced Organic Spectroscopy		4
2	MSCC2402	AdvancedBio-Inorganic	4-1-0	4
2		Chemistry	4-1-0	4
3	3MSCS2401Seminar4MSCC2403Chemistry Laboratory 45MSCP2401Project/Dissertation		0-0-4	4
4			0-0-3	4
5				8
		Total		24

#### Syllabus Semester-I

#### MSCC1101 Advanced Physical Chemistry -I

Code	Course Title	Course Type	Credits	L-T-P
MSCC1101	Advanced Physical Chemistry I	Theory	4	4-1-0

#### Module –I: Chemical Dynamics

Methods of determining rate laws, Derivation of collision theory of reaction rates, steric factor, activated complex theory, steady state kinetics, kinetic and thermodynamic control of reactions. Treatment of unimolecular reactions.

Dynamics chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen -bromine and hydrogen - chlorine reactions) and oscillatory reactions (Belousov-Zhabotinski reaction), homogeneous catalysis, kinetics of enzyme reactions. General features of fast reactions, relaxation method. Flash photolysis and the nuclear magnetic resonance method.

#### Module-II: Surface Chemistry

#### (A) Adsorption:

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation). Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electrokinetic phenomenon), catalytic activity at surfaces.

#### (B) Micelles:

Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants counter ion binding to micelles, thermodynamics of micellization, phase separation and mass action models, solubilisation, micro emulsion, reverse micelles.

#### Module-III: Electrochemistry

Derivation of electrocapiliarity; Lippmann equations (surface excess), methods of determination, Structure of electrified. Interfaces, Over potentials, exchange current density, derivation of Butler-Volmer equation, Tafelplol Quantum aspects of charge transfer at electrode - solution interfaces, quantization of charge transfer, tunnelling. Semiconductor, interfaces-theory of double layer at 14semiconductor-electrolyte solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interface. Electro catalysis-influence of various parameters, Hydrogen electrode. Bioelectrochemistry, Theresholdmembrance phenomena, Nerst-Planck equation, Hodges-Huxley equations, core conductor models, electrocardiography. Polarography theory, Ilkovic equation; half wave potential and its significance.

#### **Books Recommended:**

- 1. Physical Chemistry: P.W. Atkins, J.D. Paula, Oxford III University Press.
- 2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill, 1997, 4<sup>th</sup> edition, New Delhi.
- 3. Quantum Chemistry, Ira N. Levine, Pearson, 2007, 5<sup>th</sup> edition, New Delhi.,
- 4. Quantum Chemistry, D. A. McQuarrie and J. D. Simon, Viva, 2007, 1st edition, New Delhi.
- 5. Coulson's Valence: R Mc Weeny, ELBS.
- 6. Chemical Kinetics: K.J.Laidler, McGraw-Hill.
- 7. Kinetics and Mechanism of Chemical Transformation: J.Rajaraman and J.Kuriacose, Mcmillan.
- 8. Micelles, Theoretical and Applied Aspects, V.Moroi, Plenum.
- 9. Modem Electrochemistry: Vol.-I and Vol. II, J.O.M. Bockris and A.K. N. Reddy, Plenum.

#### [14 Hrs.]

#### [15Hrs.]

[16 Hrs.]

MSCC1102 Advanced Inorganic Chemistry –I				
Code	Course Title	Course Type	Credits	L-T-P
MSCC1102	Advanced Inorganic Chemistry I	Theory	4	4-1-0

#### **Module-I**

#### **Metal-Ligand Bonding**

Crystal Field Theory and its limitations, Elementary idea of Angular overlap model, Molecular orbital theory for octahedral, tetrahedral and square planar complexes,  $\sigma$  and  $\pi$  bonding in molecular orbital theory.

#### Module -II

#### **Electronic Spectra and Magnetic Properties of Transition Metal Complexes.**

Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes  $(d^1 - d^9 \text{ states})$ , calculations of Dq, B and racha parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereo-chemical information, anomalous magnetic moments, magnetic exchanges coupling and spin crossover.

#### **Module-III**

#### Metal -Ligand Equilibria in Solution

Type of complex equilibria in solution and types of complex equilibrium constant, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

#### **Books Recommended:**

1. Advanced Inorganic Chemistry: F.A, Cotton and G. Wilkinson, John Wiley.

- 2. Inorganic Chemistry: J.E. Huheey, E.A Keiter, RL. Keiter, Pearson Education.
- 3. Inorganic Electronic Spectroscopy: AB. P. Lever, Elsevier.
- 4. Magnetochemistry, RL. Carlin, Springer Verlag.
- 5. Comprehensive Coordination Chemistry eds.,-G. Wilkinson, RD. Gillars and J.A. McCleverty, Pergamon.
- 6. Chemical Application of Group Theory: FA Cotton, John Wiley.
- 7. Symmetry in Chemistry: Orchin and Jaffe.
- 8. Group theory: I.V. Raman, Tata McGraw Hill.

9. Group Theory & its Applications to Chemistry: KV. Raman, Tata McGraw Hill Publishing Company, New Delhi.

MSCC1103 Advanced	Organic Chemistry-I

Code	Course Title	Course Type	Credits	L-T-P
MSCC1103	Advanced Organic Chemistry I	Theory	4	4-1-0

#### Module-I

#### Nature of Bonding in Organic Molecules

Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, annulenes, antiaromaticity, homo-aromaticity, energy level of  $\Psi$ -molecular orbitals, bond order, stability.

#### **Energetics, Structure and Reactivity:**

Types of mechanism, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin - Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.

#### **Module-II**

#### **Aliphatic Nucleophilic Substitution**

The SN2, SN1, mixed SN1 and SN2 and SET mechanisms. The neighbouring group mechanism, neighbouring

[10 Hrs.]

[15 Hrs.]

## [15 Hrs.]

#### [20 Hrs.]

# group participation by $\pi$ and $\sigma$ bonds, anchimeric assistance. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambident nucleophile, regioselectivity.

#### Aromatic Nucleohilic Substitution

The SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity- effect of substrate structure, leaving group and attacking nucleophile. The Von Richter, Sommelet-hauser, and Smiles rearrangements.

#### Aliphatic Electrophilic Substitution

Bimolecular mechanisms ( $S_E2$ ) and  $S_Ei$ . The  $S_E1$  mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

#### Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, vilsmeier reaction, Gattermann-Koch reaction.

## Module-III

## [15 Hrs.]

## Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselecticity, orientation and reactivity, Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

## **Elimination Reactions**

The E2, E1 and E1cB mechanism and their spectrum. Orientation of the double bond. Reactivity – effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination. Chugaev reaction

#### **Books Recommended:**

- 1. Advanced Organic Chemistry; Reactians Mechanism and Structure: Jerry March, John.Wiley.
- 2. Advanced Organic Chemistry: F A Carey and R J. Sundberg, Plenum.
- 3. A Guide Book to Mechanism in Organic Chemistry: Peter Sykes, Longman/Pearson Education.
- 4. Structure and Mechanism in Organic Chemistry: C K Ingold, Cornell University Press.
- 5. Organic Chemistry: R. T. Marrisan and R. N Boyd, Pentice- Hall/Pearson Education.
- 6. Modern Organic Reactions: H.O. House, Benjamin.

7. Principles of Organic Synthesis: R.O.C. Norman and J.M. Coxon, Blackie Academic & Professianal/ C.B.S. Publishers.

- 8. PericyclicReactions : S.M. Mukherji. Macmillan, India Ltd.
- 9. Reaction Mechanism in Organic Chemistry: S..M. Mukherjee and S.P. Singh, Macmillian. India. Ltd.
- 10. Organic Chemistry: J. Clyden, N. Grieves, S. Warren and P.Wather, Oxfard University Press.

11. Organic Reactions and Orbital Symmetry: T.L Gilchrist and R. C. Storr, Cambridge at the University Press.

12. Photo Chemistry and PericyclicReactions :Jagdamba Singh and Jaya Singh, New Age Internatianal.

13. Mechanism and Theory in Organic Chemistry: Thomas H. Lowry, Additian Wesley.

- 14. Stereochemistry by Eliel.
- 15. Stereochemistry by P.S.Kalsi
- 16. Stereochemistry by Nasipuri.

#### MSCC1104 Polymer Chemistry

Code	Course Title	Course Type	Credits	L-T-P
MSCC1104	Polymer Chemistry	Theory	4	4-1-0

#### Module I

Kinetics of melting, crystal morphology, free volume, distribution of molecular size, stoichiometric imbalance. X-ray diffraction study, Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance

#### Module II

Price - Alfrey equation, Flory - Huggins theory, polymer fractionation, Mark - Houwink - Sakurada equation, diffusion coefficient and friction factor.

#### **Polymer Processing**

Plastics, elastomers and fibres. Compounding. Processing techniques: Calendering, die casting, rotational castin, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning. Biomedical polymers - contact lens, dental polymers, artificial heart kidney, skin and blood cells

#### Module III

Elastic deformation, shear modulus and compliances, Maxwell model, Voigt model, dynamic viscoelasticity, molecular theory for viscoelasticity - Rouse model, Coefficient of viscosity, viscosity measurement, Power Law for pseudoplastic liquids, effect of shearing forces, segmental friction factor, Bueche theory.

#### **Recommended Books**

1. Gedde Ulf. W. Polymer Physics, Chapman & Hall London (1995)

2. Rodriguez, Ferdinand, Principles of Polymer Systems Mc. Craw - Hill, International BookCo. International Student Edn. 1985.

3. Cowie; JMG Polymers: Chemistry & Physics of Modern Materials, Nelson Thornes Itd.Chelterham, 2001

4. Hiemenz; Paul C. Polymer Chemistry- The Basic Concepts; Marcell&Deckker, Inc. New York (1984)

5. Polymer Science by V.R.Gowarikar, N.V.viswanathan and J.Sreedhar, New Age International.

6. Text book of Polymer science: F.M.Billmeyer, John wiley and sons.

#### MSCC1105 Chemistry Laboratory – I

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Code	Course Title	Course Type	Credits	L-T-P
MSCC1105	Chemistry Laboratory 1	Practice	4	0-0-6

#### **Inorganic Chemistry Practical-I**

1. Qualitative analysis of mixtures containing not more than six radicals, (organic acid radicals should be excluded, less common metal ions Mo, W, Ti, V, Zr, U (two metal ions in cationic / anionic forms), insolubleoxides, sulphates and halides may be included]

2. Separation of cations and anions by (a) paper chromatography and column chromatography (b) ion exchange technique.

#### **Organic Chemistry Practical-I**

#### **Qualitative Analysis**

Identification of unknown organic compounds, separation, purification and identification of compounds of binary mixture (both are solids, one liquid & one solid) using TLC & column chromatography, Chemical tests. IR spectra to be used for functional group identification

#### **Books Recommended:**

1. Vogel'-s Qualitative Inorganic Analysis (revised) : G. Svehla, Longman.

2. Inorganic Experiments: J. DerckWoollins, VCH.

3. Microscale Inorganic Chemistry: Z. Szafran, RM. Pike and M.M: Singh, Wiley.

#### [14 **Hrs.**]

[12 **Hrs.**]

#### [15 Hrs.]

- 4. Practical Inorganic Chemistry: G. Marr, B.W. Rockett Van Nostrand.
- 5. Experiments and Techniques in Organic Chemistry, D.Pasto, C.Johnson, & M.Miller, Prantice Hall.
- 6. Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold (Publisher).
- 7. Hand Book of Organic Analysis, Qualitative & Quantitative, M.T. Clarke, Edward Arnold (Publisher).
- 8. Vogel's Text Book of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
- 9. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.
- 10. A Text Book of Practical Organic Chemistry (Qualitative). Arthur I. Vogel.

#### **Skill Elective Subject**

#### SBFE3127 Water Ouality Analysis

Code	Course Title	Course Type	Credits	L-T-P
SBFE3127	Water Quality Analysis	Practice	4	0-0-3

#### Water Quality Analysis

- a. Determination of PH of water
- b. Determination of Turbidity of water
- c. Determination of Acidity of water
- d. Determination of Alkalinity of water
- e. Determination of Hardness
- f. Determination of Dissolve Oxygen
- g. Determination of Reduction in Dissolve Oxygen
- h. Determination of Iron content of sample water
- i. Determination of Chloride ion of Water Sample
- Determination of Total Residual Chlorine in water sample j.

#### **MSCC1001** Pharmaceutical Chemistry

Code	Course Title	Course Type	Credits	L-T-P
MSCC1001	Pharmaceutical Chemistry	Practice	4	0-0-3

- 1. Extraction of Plant materials
- 2. Isolation and Identification of Phyto constituent by Preparative TLC
- 3. Isolation and Identification of Phyto constituent by Column Chromatography
- 4. Molecular Modeling and Geometry optimization of organic compounds.
- 5. Structure Search and identification by Chemspider.
- 6. In-Silico Molecular property determination of organic compounds

#### Semester-II

MSCC1201 Advanced Physical Chemistry-II				
Code	Course Title	Course Type	Credits	L-T-P
MSCC1201	Advanced Physical Chemistry II	Theory	4	4-1-0

#### **Module-I**

#### **Electronic Structure of Atoms:**

Electronic configuration. Russell-Saunders terms and coupling schemes, magnetic effects: spin-orbit coupling and Zeeman splitting.

#### **Classical Thermodynamics**

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significance. Determination of these quantities. Concept of fugacity and determination of fugacity. **Module-II** 

[10 Hrs.]

#### [04 Hrs.]

#### [10 Hrs.]

[12 Hrs.]

# Non-ideal systems:

Activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients, ionic strength.

#### **Statistical Thermodynamics:**

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging, Partition functions-translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition function. Applications of partition functions. Heat capacity behaviour of solids - chemical equilibria and equilibrium constant in terms of partition functions,

#### Module-III

#### **Quantum Chemistry**

#### **Introduction to Exact quantum Mechanical Results**

Postulates of quantum mechanics, Schrodinger equation and discussion of solutions of the Schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotator, the hydrogen atom.

#### **Approximate Methods**

The variation theorem, linear variation principle. Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

#### **Angular Momentum**

Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular moments, spin, antisymmetry and Pauli exclusion principle.

#### **Molecular Orbital Theory**

Huckel's theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. Introduction to extended Huckel theory.

#### **Books Recommended**

1. Atkin's Physical Chemistry: P.W. Atkins, J.D. Paula, Oxford University Press

- 2. Introductory to Quantum Chemistry: 4th Ed., AK Chandra, TataMcGraw Hill.
- 3. Quantum Chemistry: Ira N. Levine, Prentice Hall.
- 4. Coulson's Valence: R Mc Weeny, ELBS.
- 5. Physical Chemistry Vol-II: .RL. Kapoor, Mcmillan Publication.
- 6. Statistical Thermodynamics: M.C Gupta, New Age Pvt Publication.
- 7. Fundamentals of Molecular Spectroscopy: C.N. Banwell, McGraw-Hill.
- 8. Basic Principles of Spectroscopy: R. Chang, McGraw Hill.
- 9. Theory and Applications of U.V. Spectroscopy: H.H. Jaffe and M. Orchin, IBH- Qxford.
- 10. Quantum Chemistry: R K Prasad.

#### MSCC1202 Advanced Inorganic Chemistry-II

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Code	Course Title	Course Type	Credits	L-T-P
MSCC1202	Advanced Inorganic Chemistry II	Theory	4	4-1-0

#### **Module-I**

#### Metal $\pi$ -Complex.

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine and ligands.

#### **Metal Clusters:**

Higher boranes, carboranes, metalloboranes and, metallocarboranes. Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

#### Module –II **Organometallic Chemistry:**

#### [10 Hrs.]

[04 Hrs.]

#### [12 Hrs.]

18-Electron Rule, Ligands in Organomettallics, Synthesis, bonding and reactions of Alkyl, Aryl, Alkylidenes, Alkylidynes, Allyl, Dienyl, Arene & Trienyl complexes, Cyclic p systems (3 to 8 membered rings) and Fullerene complexes. Spectral analysis of Organometallic Complexes.

#### Module-III

#### Symmetry and Group Theory in Chemistry

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Generators, Point symmetry group.

Representations of group operators, the great orthogonality theorem (without proof) and its explanation. Irreducible and reducible representation. Bases of representation, Character of a representation. Character table and its meaning. Reduction formula.

#### **Books Recommended:**

1. Advanced Inorganic Chemistry: A Comprehensive Text: FA Cotton and G. Wilkinson, John Wiley.

2. Inorganic Chemistry: Principles of Structure and Reactivity: J.E. Huheey, E.A. Keiter and R.L. Keiter, Addition Wiley Publishing Company.

3. Comprehensive Coordination Chemistry eds.: G. Wilkinson, R.D. Gillars and JA McCleverty, Pergamon.

4. Inorganic reactions by Basalo and Pearson.

5. Spectroscopy, S. Walker and H. Straw, Chapman and Hall ltd.

6. Energy levels in atom and molecules, W.G. Richards and P.R. Scott, Oxford University Press, Oxford Chemistry Primer vol. 26, 1994, New York.

7. Atomic Spectra, T.P. Softley, Oxford University Press, Oxford Chemistry Primer, Vol. 19, New York.

8. Introduction to Spectroscopy, Pavia, Brooks/Cole Cenage, 4<sup>th</sup> edition, 2009, Belmont.

9.Symmetry and Spectroscopy of Molecules, , K.V. Reddy, New Age International (P) Ltd., Ist edition, 1998, New Delhi.

9.Fundamental Concepts of Inorganic Chemistry, A. K. Das and M. Das, Vol. 7,1<sup>st</sup> edition, 2014, CBS Publisher Pvt. Ltd., New Delhi.

10. Electronic Absorption Spectroscopy and Related Techniques, D. Sathyanarayana, University Press (India) Ltd., 2001, Hyderabad.

11. Molecular Spectrocopy, P.S. Sindhu, Tata McGraw Hill, 1985, New Delhi.

12. Fundamental of Molecular Spectroscopy, C. N. Banwell and E. McCash, Tata McGraw Hill, 4<sup>th</sup> edition, 1994, New Delhi.

#### MSCC1203 Advanced Organic Chemistry-II

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Code	Course Title	Course Type	Credits	L-T-P
MSCC1203	Advanced Organic Chemistry II	Theory	4	4-1-0

#### Module-I

#### Organic Synthesis and retrosynthesis

Synthetic design: Introduction, Retrosynthetic approach, Terminology in Retro synthetic analysis, One group disconnection, (alcohol, carbonyl compound, olefins and acids), Two group disconnections (beta-hydroxy compounds, alpha, beta-unsubstituted carbonyl compounds, 1, 3-dicarbonyl compounds, 1, 5 dicarbonyl compounds), Synthesis of some organic molecules by disconnection approach.

Organometallics in synthesis: Organo lithium, organo copper compounds, organoboranes, organometallic compounds of Zinc, Cadmium and mercury organo palladium compounds.

#### Rearrangements

General mechanistic considerations: nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements:

Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-villiger, Shapiro reaction.

#### [12 Hrs.]

[15Hrs.]

**Nuclear reaction** [08 Hrs.] Introduction, Production of projectiles, nuclear cross section, nuclear dynamics, threshold energy of nuclear

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.

Elements of symmetry, chirality, molecules with more than one chiral center, three and erythro isomers, methods of resolution, optical purity, enantiotropic and diastereotropic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes),

#### **Photochemistry:**

First order Photo chemical processes, Photo reactions: Dissociation, Reduction, Isomerisation, cycloaddition, Paterno-Buchi reaction, Norrish type-I & II reactions, Di-Pi methane reaction, Photochemistry of Arenes.

#### Module-III

#### **Pericyclic Reactions.**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3–butadiene, 1,3,5–hexatriene and allyl system. Classification of pericyclic reactions. Woodward - Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions – conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions – antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3-dipolar cycloadditions and cheletropic reactions.

Sigmatropic rearrangements - suprafacial and antarafacial shifts of H, sigmatroic shifts involving carbon moieties, 3, 3- and 5, 5-sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements. Ene reaction.

#### **RECOMMONDED BOOKS**

- 1. Modern synthetic reactions-(Benjamin) H. O. House.
- 2. Reagents in organic synthesis-(John Wiley) Fieser and Fieser
- 3. Principles of organic synthesis-(Methuen) R. O. C. Norman
- 4. Hydroboration- S. C. Brown.
- 5. Advances in Organometallic Chemistry- (A.P.)F. C. A. Stone and R. West.
- 6. Organic Chemistry (Longman) Vol. I & Vol. II- Finar
- 7. Oxidation by-(Marcel Dekker) Augustin
- 8. Advanced Organic chemistry 2nd Ed. R R. Carey and R. J. Sundburg.
- 9. Tetrahydron reports in organic chemistry- Vol.1, No. 8.
- 10. Organic Synthesis-(Prentice Hall) R. E. Ireland.
- 11. Homogeneous Hydrogenation-(J. K.) B. R. James.
- 12. Comprehensive Organic Chemistry- (Pargamon) Barton and Ollis.
- 13. Organic reactions- various volumes- R. Adams.
- 14. Some modern methods of Organic synthesis-(Cambridge) W. Carruthares.

#### **MSCC1204 Nuclear Chemistry**

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Code	Course Title	Course Type	Credits	L-T-P
MSCC1204	Nuclear Chemistry	Theory	4	4-1-0

#### **Module-I**

#### Systematic Study of alpha, beta and gamma decays

Alpha decay, energy curve, spectra of alpha particles, Giger-Nuttal law, theory of alpha decay, penetration of potential barrier, potential barrier, potential well, beta decay, range of energy relationship, beta spectrum, sergeants curve, Fermi theory of beta decay, matrix elements, allowed and forbidden transitions, curie plots, gamma decay, Nuclear energy levels, selection rule, isomeric transitions, Internal conversion, Auger effect.

#### **Nuclear Structure and Stability**

Binding energy, empirical mass equation, the nuclear models, the shell model, nuclear spin, parity & magnetic moments of odd mass numbers nuclei.

#### Module-II

#### [15 Hrs.]

[19 Hrs.]

[08 Hrs.]

reaction, formation of a compound nucleus, Nuclear reactions, direct Nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions.

#### Nuclear fission

Liquid drop model of fission, fission barrier and threshold, fission cross section, mass energy and charge distribution of fission products, symmetric and A symmetric fission, decay chains and delayed neutrons.

#### Module-III

#### **Reactor Theory**

Nuclear fission as a source of energy, Nuclear chain reacting systems, critical size of a thermal reactor, research reactors, graphite moderated, heterogeneous, enriched uranium reactors, light water moderated, heterogeneous, enriched uranium reactors, water boilers enriched aq. Homogeneous reactors, Thermonuclear reactors, gamma interactions, shielding and health protection. Reactors in India.

#### **Recommended Books.**

- 1. Friedlander, Kennedy and Miller, Nuclear and Radio Chemistry: John Wiley
- 2. B.G. Harvey, Nuclear Chemistry
- 3. Hassinsky: Translated by D.G. Tuck, Nuclear Chemistry and its application: Addison Wiley
- 4. B.G. Harvey, Introduction to Nuclear Physics and Chemistry
- 5. Maeclefort: Nuclear Chemistry: D.VanNostrand
- 6. An N.Nesmeyannoy: Radiochemistry: Mir
- 7. Jacobs et al: Basic Principles of nuclear Science and Reactors, V.Nost & EWAP
- 8. N.Jay: Nuclear Power Today Tomorrow: ELBS
- 9. Kenneth: Nuclear Power Today, Tomorrow: ELBS
- 10. Essentials of Nuclear Chemistry, W.J. Arnikar, John Wiley
- 11. Nuclear and Radiation Chemistry: B.K. Sharma, Krishna Publication
- 12. An Introduction to Nuclear Physics: R. Babber. And Puri.

#### MSCC1205 Chemistry Laboratory 2

Code	Course Title	Course Type	Credits	L-T-P
MSCC1205	Chemistry Laboratory 2	Practice	4	0-0-6

#### **Organic chemistry practical-III**

Organic synthesis

- 1. Estimation of sulphur, nitrogen and functional groups, pharmaceutical analysis.
- 2. Polyfunctional analysis of organic compounds
- 3. Organic preparations
  - i. Preparation of anthranilic acid
  - ii. Preparation of phthalimide
  - iii. Preparation of N- bromosuccinamide
  - iv. Preparation of p- Amino benzoic acid
  - v. Preparation of p- chloro nitrobenzene by Sandmeyer reaction
  - vi. Preparation of p- Idonitrobenzene by Sandmeyer reaction
  - Vii. Pinacol- Pinacolone rearrangement

#### **Inorganic Chemistry Practical-II**

Recommended Books:

- 1. A Textbook of Practical Organic Chemistry A. I. Vogel.
- 2. Practical Organic Chemistry Mann & Saunders.
- 3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke.
- 4. Organic Synthesis Collective Volumes.
- 5. Organic Reactions (Wiley).

#### [07 Hrs.]

#### **Skill Elective-2**

#### SBFE3152 Clinical Practice Lab

Code	Course Title	Course Type	Credits	L-T-P
SBFE3152	Clinical Practice lab	Practice	4	0-0-3

Content of Experiment

- 1. General consideration on specimen collection in the Lab (Blood, Stool, Urine, sputum pus, semen)
- 2. Routine examination of urine sample albumin, sugar, bile salt, bile pigment, ketone body
- 3. Detection of HCG (Hormonal Test)
- 4. Detection of Blood Glucose and cholesterol
- 5. Estimation of hemoglobin, DLC, Blood group and total lymphocyte count.

#### MSCC1002 Analytical Chemistry

Code	Course Title	Course Type	Credits	L-T-P
MSCC1002	Analytical Chemistry	Practice	4	0-0-3

#### Analysis of soil:

Composition of soil, Concept of pH and pH measurement, Complexometric titrations, Chelation, Chelating agents, use of indicators

a. Determination of pH of soil samples.

b. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration

#### Analysis of food products:

Nutritional value of foods, idea about food processing and food preservations and adulteration.

a. Identification of adulterants in some common food items like coffee powder, asafetida, chilli powder, turmeric powder, coriander powder and pulses, etc.

b. Analysis of preservatives and colouring matter.

#### **Chromatography:**

Definition, general introduction on principles of Chromatography, paper chromatography, TLC etc.

a. Paper Chromatographic separation of mixture of metal ion ( $Fe^{3+}$  and  $Al^{3+}$ ).

b. To compare paint samples by TLC method

#### **Recommended Books:**

1. Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. Instrumental Methods of Analysis, 7th Ed. Wadsworth

Publishing Company Ltd., Belmont, California, USA, 1988.

2. Skoog, D.A., Holler, F.J. & Crouch, S. *Principles of Instrumental Analysis*, Cengage Learning India Edition, 2007.

#### Semester-III

#### MSCC2301 Advanced Inorganic Chemistry III

	8	2		
Code	Course Title	Course Type	Credits	L-T-P
MSCC2301	Advanced Inorganic Chemistry III	Theory	4	4-1-0

#### Module I

#### Instrumental Method of Analysis:

#### [8 Hrs.]

Atomic absorption and Flame emission spectral method and their application in quantitative analysis. Molecular absorption and emission spectroscopy in quantitative analysis. Light scattering technique including nephlometry

Magnetic hyperfine interaction.

#### Module II

#### Homogeneous and Heterogeneous Catalysis:

Stoichiometric reactions for organometallic catalysts: Dissociation & Substitution, Oxidative addition & carbonylation, Oxygen transfer from Peroxo and Oxo Species, Reductive & Hydride elimination, Insertion, Displacement and Isomerization reaction. Hydrogenation, Hydroformylation, Wacker (Smidt) Process, Olefin Metathesis, Fischer-Tropsch synthesis, Zeigler-Natta polymerization, Water gas reaction.

#### Module III

#### **Mechanism of Substitution Reactions:**

The nature of substitution reactions, Kinetic Application of Crystal Field Theory. Acid hydrolysis of octahedral Co (III) complexes with reference to effect of charge, chelation, steric crowding & effects of leaving group. Base hydrolysis of octahedral Co(III) complexes: Conjugate base mechanism, Test of conjugate base mechanism. Anation reaction.

#### **Electron Transfer Reactions:**

Introduction, electron tunneling hypothesis, Marcus-Hush theory, atom transfer reactions, one and two electron transfer, inner sphere and outer sphere reaction, electron transfer through extended bridges and the hydrated electron.

#### **Recommended Books:**

- Spectroscopy Vol. I & II: Walker & Straw.
- Fundamentals of Molecular Spectroscopy: C.N. Banwell.
- Molecular Spectroscopy: P.S. Sindhu.
- Fundamentals of Molecular Spectroscopy: G.M. Barrow.
- Mechanisms of Inorganic Reactions: F. Basolo and R.G. Pearson. •
- Inorganic Chemistry: Cotton and Wilkinson (4th Ed).

MSCC2302 Advanced Organic Chemistry III (Biomolecules)						
Code	Course Title	Course Type	Credits	L-T-P		
MSCC2302	Advanced Organic Chemistry III	Theory	4	4-1-0		

#### **Module-I**

#### **Bioenergetics**

Standard free energy change in biochemical reaction Exergonic, Hydrolysis of ATP, Synthesis of ATP from ADP.

#### **Amino Acids, Peptides and Proteins:**

Classification and functions of amino acids and proteins, Chemical reactions of amino acids, alkali titration of amino acids, Synthesis of peptides,  $\alpha$ -helix,  $\beta$ -sheets, super secondary structure, triple helix structure of collagen. Primary, secondary, tertiary and quaternary structures of proteins. Tertiary structure of proteinfolding and domain structure. Quaternary structure.

Module II

#### Enzymes

#### **Raman Spectroscopy:**

Classical and quantum theories of Raman Effect pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, Mutual exclusion principle. Resonance Raman Spectroscopy (RRS), Coherent Antistokes Raman Spectroscopy (CARS).

#### **Electron Spin Resonance Spectroscopy:**

Theory, instrumentation, g-values, hyperfine splitting, ESR spectra of systems with more than one unpaired electrons, double resonance, ENDOR and ELDOR techniques.

#### **Mossbauer Spectroscopy:**

Principles of Mossbauer spectroscopy, Experimental methods, Theoretical aspects, Quadrupole splitting,

#### [5 Hrs.]

#### [8 Hrs.]

[10 Hrs.]

## [15 Hrs.]

#### [15 Hrs.]

#### [10 Hrs.]

Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis

#### Module III

Purine and pyrimidine of nucleic acids, base pairing via H–bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. Overview of Replication, Transcription and Translation processes, Sequencing of nucleic acids, Genetic code, Recombinant DNA.

#### **Recommended Books:**

- 1. Principles of Biochemistry, A. L. Lehinger, Worth Publications.
- 2. Biochemistry, Voet and Voet, John Wiley.

#### MSCC2303 Advanced Physical Chemistry III

Code	Course Title	Course Type	Credits	L-T-P
MSCC2303	Advanced Physical Chemistry III	Theory	4	4-1-0

#### Module I

#### **Electronic spectra of molecule:**

Introduction, Absorption of light; The Beer–Lambert Law and its deviation, relation between molar extinction coefficient and absorption cross section, Electronic spectra of diatomic molecules: The Born-Oppenheim Approximation, vibrational coarse structure, intensity of Vibrational-electronic spectra: the Franck–Condon principle, notation of energy levels and electronic transitions, Electronic spectra of polyatomic molecules: auxochromo and chromophore, Selection rules, applications.

#### Nuclear Magnetic Resonance Spectroscopy:

Introduction, Theory of Nuclear magnetic resonance, chemical shift, factors affecting chemical shift, spin-spin splitting, Advanced NMR techniques, Application of NMR

#### Module II

## Photophysical Chemistry I:

Fluorescence:

Introduction, principles and instrumentation; choice of light sources, monochromators, choice of optical filters and various detector systems used, Jablonski Diagram, Characteristics of Fluorescence Emission, Fluorescence Lifetimes and Quantum Yields, Stoke's shift, fluorescence excitation spectrum, Fluorescence Anisotropy. Effects of solvents on the fluorescence spectrum: (general effects and specific effects, derivation of the equation, Temperature Effects)

#### Module III

#### Photo physical Chemistry II:

Fluorescence quenching and Resonance Energy Transfer: Different mechanism of fluorescence quenching & applications, Different mechanisms of energy transfer (Forster and Dexter mechanism), selection rules for energy transfer, non-vertical energy transfer, Forster Resonance Energy Transfer (FRET), typical examples and choice of dyes and applications.

#### Data analysis:

Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

#### **Recommended Books:**

- Chemical application and group Theory; F.A. Cotton, 3rd edition (1999).
- Fundamentals of Photochemistry; K. K. Rohatagi-Mukherjee.
- Molecular Fluorescence: Principles and Applications; Bernard Valeur.
- Principles of Fluorescence Spectroscopy; Springer; 3rd edition (2006), J. R. Lakowicz.

#### [15 Hrs.]

## [18 Hrs.]

#### [10 Hrs.]

[16 Hrs.]

#### [6 Hrs.]

Basic Principle of Analytical Chemistry; S.M. Khopkar.

Wibee2504 Mavaneed Bona State Chemistry						
Code	Course Title	Course Type	Credits	L-T-P		
MSCC2304	Advanced Solid State Chemistry	Theory	4	4-1-0		

MSCC2304 Advanced Solid State Chemistry

#### Module I

#### **Crystal Structure**

(a) Crystal lattice, Crystal planes, Miller indices, Bragg's law, Determination of crystal structure (NaCI, KCI, ZnS, and CsCl), Structure of elements and compounds.

(b) Bonding in Solids: Vander waal's force, force of covalency, bonding in ionic solids, Born-Harber cycle, theoretical evaluation of lattice energy, imperfections in solids, Schottky and Frenkel defects.

#### Module II

#### **Electronic structure of solids-band theory:**

Band structure of Solid: Metals and their properties; semiconductors: Intrinsic and extrinsic semiconductors, Fermi Levels; Hall Effect, Semiconductors devices: p-n junctions and other devices; insulators-dielectric, ferroelectric, pyroelectric and piezoelectric properties; ionic conductors.

Mechanical Properties of Solids: Stress, strain, deformation, tensile properties, ductility, and other mechanical properties of metals

**Magnetic properties**: Dia, para, ferro, ferri, and antiferro magnetic types; soft and hard magnetic materials; magnetoresistance.

#### **Organic Solids**

Electrically conducting solids, organic charge transfer complex, organic metals, new superconductors.

#### **Module III**

**Diffraction Methods** 

#### **X-ray Diffraction**

Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, indexing, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices, and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, Ramchandran diagram.

#### **Neutron Diffraction**

Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

#### **Recommended Books:**

- Solid State Chemistry by D. K. Chakravarty. •
- Solid State Chemistry and its Applications by R. West, John Wiley & Sons, 1984.
- Solid State Chemistry An Introduction by L. Smart and E. Moore, Chapman & Hall, 1992. •
- Principles of the Solid State by H. V. Keer, Wiley Eastern Limited, 1993.
- Solid State Chemistry by K. Chakrabarty, New Age Publishers, 1996. •
- Principles of Materials Science and engineering, Navneet Gupta, 2<sup>nd</sup> Ed, Dhanpat Rai & Co. •
- Applications of Neutron Powder diffraction, E.H. Kisi and C.J. Howard, Oxford Science, 2008, New • York.
- Introduction to Solid State Physics, C. Kittel, John Wiley, 1976, New York .Elements Of X Ray • Diffraction, B. D Cullity, Addison-Wesley Publishing Company Inc., 1956, USA.

#### [15 Hrs.]

# [12 Hrs.]

# [15 Hrs.]

<b>MSCC2305</b>	Chemistry	Laboratory -3
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Code	Code Course Title		Credits	L-T-P
MSCC2305	Chemistry Laboratory 3	Practice	4	0-0-6

#### **Physical Chemistry Practical**

- 1. Determination of ionization constants of weak acids and verification of Oswald's Dilution law.
- 2. Verification of Onsager's limiting law.
- 3. Conduct metric titration of a mixture of HCl+CH<sub>3</sub>COOH with NaOH
- 4. Determination of solubility product of BaSO<sub>4</sub>.
- 5. Potentiometric titration of strong acid with strong base.
- 6. Determination of temperature coefficient and energy of activation of hydrolysis of ethyl acetate.
- 7. To determine the rate constant of base hydrolysis of ester titrometrically.
- 8. pH meter: Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid.
- 9. To study the simultaneous equilibria in benzoic acid benzene- water system.
- 10. Conductometry: Hydrolysis of NH<sub>4</sub>Cl or CH<sub>3</sub>COONa or aniline. Hydrochloride, Determination of dissociation constant of acetic acid, Hydrolysis of ethyl acetate by NaOH.

#### **Reference Books:**

- Experimental Physical Chemistry: RC Das and B Behera
- Practical physical chemistry: B Viswanathan and P.S .Raghavan
- Practical chemistry: Vogel

#### **MSRM5101 Introduction to Research**

Code	Course Title	Course Type	Credits	L-T-P
MSRM5101	Introduction to research	Theory	2	2-0-0

#### Module-I: (13Hrs)

**Research: Introductory Concepts:** Curiosity and Research, Common sense vs. Sciences, Role of Observation and Scientific Methods, Experiments as the basis of Sciences, Various types of Research Methods in Sciences, Discussion of various research methods.

**Overview of Research Process:** Problem Definition, Proposition of Hypotheses, Hypothesis Testing, Types of Possible Errors in Hypothesis Testing, Proposition of Models and Theories, Literature Review, Experimental Design, Sampling and Survey, Measurement of Values and Dealing with Errors, Validation of Results, Improving Theories, Models and Experiments, Safety and Ethics.

#### Module-II: (12Hrs)

**Data Analysis-I:** Use of Statistics in Data Analysis, Probability Distributions, Central Limit Theorem and its applications in Data Analysis, Comparing many experimental measurements, Data with many values of independent variables.

**Data Analysis-II:** Building Mathematical Models, Ingredients of Mathematical Models, Estimation, Regression methods, Fourier Transforms, Interative Maps, Differential Equations.

Other Methods of Data Analysis: Tables, Graphs and Charts.

#### Module: III (5hrs)

**Documentation and Presentation:** Scientific Proposal Writing, Scientific Report Writing, Parts of a Scientific Report, Presentations, Ethical Issues in Report Writing.

#### **Text Books:**

1. Michael P Marder, 2011, Research Methods for Science, Cambridge University Press.

#### **Reference Books:**

- 1. Eugene Bright Wilson, 1991, AnIntroduction to Scientific Research, Dover Publications Inc.
- 2. Ranjit Kumar, 2011, Research Methodology: A Step by Step Guide, Sage South Asia Publication.

1.	Concepts on O	Green Che	emistry, C	Goals, ne	eds of C	Green (	Chemistry

- 2. Preparation of biodiesel from vegetable/ waste cooking oil.
- 3. Preparation of propene from 1-propanol + conc. sulphuric acid
- 4. Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide.
- 5. Extraction of D-limonene from orange peel using liquid CO2 prepared form dry ice.

Course Title

Advanced Organic Spectroscopy

- 6. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).G
- 7. Preparation and characterization of nanoparticles of gold using tea leaves.

#### Module I

#### **Ultraviolet Spectroscopy:**

Code

MSCC2401

Woodward- Fisher rules for conjugated dienes and carbonyl compounds; Calculation of  $\lambda$  max. Ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

Semester IV MSCC2401 Advanced Organic Spectroscopy

Course Type

Theory

Credits

4

L-T-P

4-1-0

[12 Hrs.]

#### **IR Spectroscopy:**

Characteristic vibrational frequencies of alkanes; alkenes; alkynes; aromatic compounds; alcohols; ethers; phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters; amides, acids, Anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies; overtones; FT-IR of gaseous; solids and polymeric materials.

#### Module II

#### Nuclear Magnetic Resonance Spectroscopy:

# The nature of spinning particles, interaction between spin and a magnetic field. Population of energy levels, the larmor precession. Relaxation times. The meaning of resonance and the resonance condition. NMR experiment, significance of shielding constants and chemical shift. The origin and effect spin - spin coupling, factors affecting chemical shift, chemical analysis by NMR. Exchange phenomena, 13C NMR spectroscopy, double resonance and nuclear-overhauser effect.

#### Module III

#### Mass Spectrometry:

Introduction, ion production, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, nitrogen rule. High-resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Structural problems based on combined spectroscopic techniques.

#### **Reference Books**

- W. Kemp, Organic spectroscopy ELBS.
- D.W. Williams and Flemming, Spectroscopic methods of organic compound.
- Silverstein and Basallar, Spectroscopic identification of organic compounds.
- P.S. Kalsi Spectroscope of organic compounds (New age publisher).
- Jafee and Orchin, Theory and application of U.V.

#### MSCC2306 Green Chemistry Lab

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Code	Course Title	Course Type	Credits	L-T-P
MSCC2306	Green Chemistry Lab	Practice	2	0-0-3

# [12 Hrs.]

#### MSCC2402 Advanced Bio-Inorganic Chemistry

Code	Course Title	Course Type	Credits	L-T-P
MSCC2402	Advanced Bio-Inorganic Chemistry	Theory	4	4-1-0

#### Module I

#### Metalloporphyrins and Iron-sulphur Protein

Iron porphyrins (Heme proteins): Hemoglobin (Hb), Myoglobine (Mb) their behavior asoxygen carrier and oxygen uptake protein,  $O_2$  affinity cooperativity and Bohr's effect, Heme protein as electron carrier with particular reference to reference to cytochrome-c and cytochrome-450, and cytochrome oxydase. Magnesium porphyrins (Chlorophyll): Photosynthesis, the light and dark reaction (Calvin cycle). Non-heme iron-sulphur protein as electron carrier, rubredoxins and ferredoxins.

#### Module II

#### Metalloenzymes

Preliminary idea about enzyme, co-enzyme and metalloenzyme, Enzyme-substrate binding problem, The Michaelis-Menten's equation, carboxypeptidase, carbonic anhydrase and their biological significance, oxydases, nitrogenases and its role in nitrogen fixation, Interchangeability of zinc and cobalt enzyme Supramolecular Chemistry: Host guest chemistry, chiral recognition and catalysis, molecular recognition, biomimetic chemistry, crown ethers, cryptates. Cyclodextrine, cyclodextrinbased enzyme models, calixarenes, Ionophores.

#### Module III

#### Supramolecular Chemistry.

Concepts and language. Molecular recognition: Molecular receptors for different types of molecules including arisonic substantes, design and synthesis of coreceptor molecules and multiple recognition. Supramolecular reactivity and catalysis.

Transport processes and carrier design. Supramolecular devices, Supramolecular photochemistry, supramolecular electronic, ionic and switching devices.

Some example of self-assembly in supramolecular chemistry.

#### **Recommended Books:**

#### Text books

- Basic Inorganic Chemistry (3rd ed): Cotton, Wilkinson & Gaus.
- Inorganic chemistry (4th Ed): Huheey, Keiter & Keiter.
- Bioinorganic and Suparmolecular Chemistry: Bhagi, G.R.Chatwal.
- Bio-Inorganic chemistry: E.Ochiai.
- Bio-Inorganic chemistry: R.W. Hay.

#### **Reference Books**

- Supramolecular Chemistry, J. W. Steed and J. L. Atwood, Willey, 2<sup>nd</sup> Ed (2009).
- Bioorganic, Bioinorganic and Supramolecular Chemistry, P.S. Kalsi, J.P. Kalsi, New Age International, 2<sup>nd</sup> Ed (2012).
- An Introduction of Supramolecular Chemistry, Asim K. Das, Books and Allied, 1st Ed (2017

MSCC2403 Chemistry laboratory-4						
Code	Course Title	Course Type	Credits	L-T-P		
MSCC2403	Chemistry Laboratory 4	Practice	4	0-0-6		

#### MSCC2403 Chemistry laboratory-4

#### Instrumental Methods of Analysis Lab

- 1. Determination of the concentration of glycine solution by formylation method.(Titration curve of glycine)
- 2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
- 3. Measurement of calorific value of food items by bomb calorimeter.
- 4. Synthesis of hydrogel by co-precipitation method.

#### [15 Hrs.]

#### [15 Hrs.]

5. Synthesis of silver and gold metal nanoparticles.

6. Determination of elemental composition of coal, iron rod etc by X-ray florescence method.

7. Determination the validity of Beer's Law by UV-Vis Spectrophotometry.

8. Identification of metal ions  $Ni^{2+}$ ,  $Fe^{3+}$ ,  $Co^{2+}$ ,  $Cu^{2+}$  by UV-Vis Spectrophotometry

9. Kinetic study of the oxidation of Ascorbic acid by hexacyano ferrate (III) ion by UV-Vis Spectrophotometry.

#### **Recommended Books**:

1. D.A. Skoog, F.J. Holler & S. Crouch (ISBN 0-495-01201-7) *Principles of Instrumental Analysis*, Cengage Learning India Edition, 2007.

2. Willard, Merritt, Dean, Settle, *Instrumental Methods of Analysis*, 7th ed, IBH Book House, New Delhi.

- 3. Atkins, P.W & Paula, J.D. Physical Chemistry, 10th Ed., Oxford University Press (2014).
- 4. Kakkar, R. *Atomic and Molecular Spectroscopy: Concepts and Applications*. Cambridge University Press, 2015.
- 5. Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
- 6. Banwell, C. N. & McCash, E. M. *Fundamentals of Molecular Spectroscopy* 4th Ed. Tata McGraw-Hill: New Delhi (2006).

MISCI 2401 I KOJECI						
Code	Course Title	Course Type	Credits	L-T-P		
MSCP2401	Project	Project	8	0-0-6		

#### **MSCP2401 PROJECT**