M.Sc. Chemistry

Year	FIRST SEMESTER						SECOND SEMESTER					
	Course Code	**Course Name**	**L**	**T**	**P**	**C**	**Course Code**	**Course Name**	**L**	**T**	**P**	**C**
I	CY6101	Chemistry of Main Group Elements	2	1	0	3	CY6201	Chemistry of Transition Metals	2	1	-	3
	CY6104	Stereochemistry, Reaction Mechanism and Aromaticity	2	1	0	3	CY6202	Analytical Chemistry and Bonding	3	1	-	4
	CY6105	Spectroscopy	3	1	0	4	CY6204	Advanced Organic Chemistry of Multiple Bonds	2	1	-	3
	CY6107	Surface Chemistry and Thermodynamics	2	1	0	3	CY6207	Quantum Chemistry, Electrochemistry and Chemical Kinetics	2	1	-	3
	CY6108	Symmetry and Group Theory	2	1	0	3	CY6230	Advanced Chemistry Laboratory - II	0	0	8	4
	CY6130	Advanced Chemistry Laboratory - I	0	0	12	6	MA6205	Research Methodology and Technical Writing	2	1	0	3
							CY6271	Student Seminar	-	-	-	1
			11	5	12	22			11	5	8	21
	Total Contact Hours (L + T + P)		**28**				**Total Contact Hours (L + T + P)**		**24**			
	THIRD SEMESTER						**FOURTH SEMESTER**					
II	CY7101	Organometallic Chemistry	2	1	0	3	CY8270	Major Project	0	0	32	16
	CY7104	Photochemistry, Pericyclic Reactions and Heterocyclic Chemistry	2	1	0	3						
	CY7107	Solid State Chemistry	2	1	0	3						
	CY7130	Advanced Chemistry Laboratory - III	0	0	6	3						
	CY71xx	**DSE - I	2	1	0	3						
	CY71xx	**DSE - II	2	1	0	3						
	CY71xx	**DSE - III	2	1	0	3						
			12	6	6	21			0	0	32	16
	Total Contact Hours (L + T + P)		**24**				**Total Contact Hours (L + T + P) + OE**		**32**			

DISCIPLINE SPECIFIC ELECTIVE (DSE)		
DSE – I [Group A (Inorganic)]	**DSE – II [Group B (Organic)]**	**DSE – III [Group C (Physical)]**
1. CY7140: Photo Inorganic Chemistry	1. CY7150: Medicinal Chemistry	1. CY7160: Computational Chemistry
2. CY7141: Bio-Inorganic Chemistry	2. CY7151: Chemistry of Biomolecules	2. CY7161: Biophysical Chemistry
3. CY7142: Nuclear and Radiochemistry	3. CY7152: Bio-Organic Chemistry	3. CY7162: Advanced Quantum Chemistry
4. CY7143: Metallurgical Science	4. CY7153: Textile Chemistry	4. CY7163: Liquid State
		5. CY7164: Catalysis Technology

FIRST SEMESTER

CY6101: CHEMISTRY OF MAIN GROUP ELEMENTS [2 1 0 3]

Stereochemistry and Bonding in Main Group Compounds: VSEPRT, hybridization, covalently bonded molecules. Hydrogen, Alkali and Alkaline Earth Metals: Hydrides, application of crown ethers. Noble Gases: Isolation and properties, preparation and structure of noble gas compounds. Boron Compounds: Boranes, carboranes, metalloboranes, metallocarboranes, borazines. Compounds of Carbon and Silicon: Fullerenes, carbon nano-tubes, carbides, fluorocarbons, silanes, silicates, zeolites and silicones. Compounds of Oxygen Group Elements: Metal selenides and tellurides, oxyacids and oxoanions of S & N. Compounds of Nitrogen Group Elements: BN, PN and SN compounds - preparation, structure and bonding. Compounds of Halogen Group Elements: Interhalogens, oxyacids and oxoanions of halogens. Reaction in Non-aqueous Solvents: Reaction in liquid ammonia, liquid sulphur dioxide, DMF, DMSO.

References:

1. D. F. Shriver, P.W. Atkins, C.H. Langford, Inorganic Chemistry, Oxford University Press, 2010.
2. G. L. Miessler, D.A. Tarr, Inorganic Chemistry, Pearson Publications, 2011.
3. G. Wulfsberg, Inorganic Chemistry, University Science Books, Viva Books Pvt. Ltd, 2013.

CY6104: STEREOCHEMISTRY, REACTION MECHANISM AND AROMATICITY [2 1 0 3]

Stereochemistry: Chirality, stereochemistry of different compounds, resolution of racemates, Stereo selectivity and stereo specificity, conformational analysis of ethane and cycloalkanes. Reaction Mechanism: Methods of determining reaction mechanism, nucleophilic substitution reactions factors affecting reactivity, elimination reactions, addition to carbon–carbon multiple bonds, radicals in organic synthesis. Aromaticity: Hückle's rule, aromatic electrophilic substitution, nucleophilic aromatic substitution, various types.

References:

1. M. J. T. Robinson, Organic Stereochemistry, Oxford University Press, 2005.
2. E. L. Eliel, S. H. Wilen, L. N. Manden, Stereochemistry of Carbon compounds, Wiley, 2005.
3. R. Bruckener, Advanced Organic Chemistry: Reaction mechanism, Elsevier, 2009.

CY6105: SPECTROSCOPY [3 1 0 4]

Spectroscopy: Rotational & vibrational spectroscopy: Intensity & width of a spectral line, rotational raman spectra, selection rules for vibrational spectrum, vibration-rotation spectra & spectral branches, electronic spectroscopy: nature of transition, fluorescence & phosphorescence, elementary ideas of laser and laser action, symmetry aspects of molecular orbital theory with examples, UV-VIS spectroscopy: Electronic levels and types of electronic transitions in organic, inorganic and organometallic systems, IR and Raman spectroscopy: FT technique, group frequencies, vibrational coupling, Raman spectroscopy. Mass spectrometry: Ion production: EI, CI, FD, FAB, ion analysis techniques. Nuclear Magnetic Resonance Spectroscopy: NMR phenomenon, spin ½ nuclei, 1H, 13C, 19F and 31P, Zeeman splitting. ESR spectroscopy: ESR phenomenon, introduction to the ESR spectra of organic free radicals and ion radicals.

References:

1. R. M. Silverstein, G. C. Bassler, T.C. Morril, Spectrometric Identification of Organic Compounds, John Wiley, New York, 2009.
2. W. Kemp, Organic Spectroscopy, 2nd edition, ELBS Macmillan, Hongkong, 2011.
3. E. A. V. Ebsworth, D. W. H. Rankin, S. Cradock, Structural Methods in Inorganic Chemistry, Blackwell Publications, London, 2013.

CY6107: SURFACE CHEMISTRY AND THERMODYNAMICS [2 1 0 3]

Surface Chemistry: Surfaces and interfaces, dispersed systems, surfactants, CMC, emulsions, colloids, vesicles, foams and aerosols. Thermodynamics: Laws of thermodynamics, reaction equilibrium, gibbs energies of pure phases and allotropes, binary solutions, partial molar properties & their significance, statistical thermodynamics, Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, derivation of distribution laws (most probable distribution) for the three types of statistics, evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases.

References:

1. P.W. Atkins, J. De Paula, Physical Chemistry, W.H. Freeman, 2012.
2. R. P. Rastogi & R. R. Mishra, An Introduction to Chemical Thermodynamics, Vikas Publishing House Pvt Ltd, 2010.
3. B.R. Puri, L. R. Sharma, M. S. Pathania, Principles of Physical Chemistry, Vishal Publishing House, 2019.
4. D. A. McQuarrie, Statistical Mechanics, Viva Books Pvt. Ltd.: New Delhi, 2013.
5. D. A. McQuarrie, Molecular Thermodynamics, Viva Books Pvt. Ltd.: New Delhi, 2010.

CY6108: SYMMETRY AND GROUP THEORY [2 1 0 3]

Symmetry: Groups, symmetry operations, symmetry elements, point groups, point group of molecules, optical activity and symmetry. Representations of Groups: Reducible & irreducible representations, unit vector transformations, character table, and general relationships of irreducible representations. Techniques and Relationships for Chemical Applications: Systematic reduction of reducible representations, IR and Raman active irreducible representations, direct product of irreducible representations

References:

1. F.A. Cotton, Chemical Applications of Group Theory, Wiley International, 2010.
2. S. Swarnalakshmi, T. Saroja, & R. M. Ezhilarasi, Simple Approach to Group Theory in Chemistry, Universities Press, 2008.
3. H. H. Jaffe, M. Orchin, Symmetry in Chemistry, Dover Publications, 2008.
4. R. L. Carter, Molecular Symmetry and Group Theory, Wiley International, 2009.

CY6130: ADVANCED CHEMISTRY LABORATORY-I [0 0 12 6]

Qualitative Analysis: Separation, purification and identification of compound of binary mixture (one liquid & one solid) using TLC & column chromatography, chemical test, IR spectra to be used for functional group identification, Organic Synthesis: Acetylation, Oxidation, Aldol Condensation, Esterification, Cannizzaro Reaction, Friedel-Crafts Reaction, Aromatic Electrophilic Substitution etc., Quantitative Analysis: Iodine and saponification values determination in an oil sample, Amines/phenols determination using bromate bromide solution/acetylation method, BOD, COD, DO estimation in given water sample etc. Error Analysis and Statistical Analysis, Phase Equilibria: Congruent composition and temperature of a binary system determination; construction of phase diagram for three component system, Chemical Kinetics: Determination of rate constant of hydrolysis of an ester/ionic reaction in micellar media, Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as iodine clock reactions, Electrochemistry: Conductrometric and pH Metric analysis.

References:

1. B. S. Furniss et al., Vogel's Textbook of Practical Organic Chemistry, Pearson Education, 2003.
2. G. Svehla, B. Sivasankar, Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012.
3. S. K. Maity, N. K. Ghosh, Physical Chemistry Practical, New Central Book Agency, 2012.
4. A. K. Srivastava, Instrumental Approach to Chemical Analysis, S Chand & Co., 2010.

SECOND SEMESTER

CY6201: CHEMISTRY OF TRANSITION METALS [2 1 0 3]

Metal-Ligand Bonding: Nomenclature and stereochemistry of compounds, valence bond theory (VBT), crystal field theory (CFT), crystal field stabilization energy (CFSE), molecular orbital theory of octahedral, tetrahedral and square planar complexes. Metal Ligand Equilibria in Solution: Factors affecting stability of metal complexes with reference to the nature of metal ion and ligand chelate effect and its thermodynamic origin. Electronic Spectra of Transition Metal Complexes: Types of electronic transition, selection rules for d-d transitions. Magnetic Properties of Transition Metals: Origin of magnetic moment, spin contribution, spin only formulas, orbital contribution, spin-spin coupling. Reaction Mechanism of Transition Metal Complexes: Energy profile of a reaction, reactivity of metal complex, inert and labile complexes. Compounds with Metal-Metal Multiple Bonds and Poly-ions: Metal carboxylate and halide compounds with metal –metal multiple bonds.

References:

1. F.A. Cotton, G. Wilkinson, C.A. Murollo and M. Bochmann, Advanced Inorganic Chemistry, John Wiley & Sons, 2009.
2. J. E. Huheey, Inorganic Chemistry, Harper & Row: New York, 2011.
3. A. B. P. Lever, Inorganic Electronic Spectroscopy, Elsevier, 2011.
4. R. D. L. Carlin, Magnetochemistry, Springer-Verlag: Berlin, 2014.

CY6202: ANALYTICAL CHEMISTRY AND BONDING [3 1 0 4]

Measurement and Data Analysis: Accuracy, precision, Significant figures, Gaussian distribution of data, standard deviation, regression analysis, least squares method, correlation coefficient. Solvent Extraction: Extraction equilibria and extraction systems - Chelation, solvation and ion-pair formation. Chromatography: Ion exchange chromatography, planar chromatography, HPLC. Spectral Methods: Bear-Lambert Law, UV-Visible Spectrophotometry Instrumentation and application, AES, Flame photometry, Fluorescence spectrophotometry. Radioanalytical Methods: Radioactivity as analytical tool. Neutron activation analysis. Thermal Methods: TGA, DTA, DSC – Basics, instrumentation and applications. Electroanalytical Techniques: Potentiometry, coulometry, polarography, cyclic voltammetry, anodic stripping, electrophoresis and its applications.

References:

1. G. D. Christian, Analytical Chemistry, 5th Edition, John Wiley &Sons, Inc, New York, 2004.
2. A. J. Bard and L. R. Faulkner, Electrochemical Methods: Fundamentals and Applications, John Wiley & Sons, 2001.

3. D. A. Skoog, D. M. West, Principles of Instrumental Analysis, Holt Rinahart Winston, New York, 2006.
4. K. A. Robinsons, Chemical Analysis, Harper Collins Publishers, New York, 2010.
5. H. A. Wiliard, L. L. Merrit, J. A. Dean, Instrumental Methods of Analysis, van Nostrand, New York, 2013.
6. P. T. Kissinger and W. R. Heineman, Laboratory Techniques in Electroanalytical Chemistry, Marcel and Dekker Publisher, 1984.

CY6204: ADVANCED ORGANIC CHEMISTRY OF MULTIPLE BONDS [2 1 0 3]

Alkenes and Alkynes: Synthesis of alkenes and alkynes, reactions of alkenes and alkynes. Carbonyl Compounds: Modern methods of synthesis from alcohols, reactions of carbonyl compounds, addition of N, O, and S nucleophiles, emphasis on synthetic utility of these reactions, rearrangement reactions involving electron deficient carbon, nitrogen, oxygen centers, the synthetic utility of these rearrangements.

References:

1. F. A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 3rd edition, Plenum Press, New York, 2010.
2. J. March, Advanced Organic Chemistry, 4th edition, Wiley Interscience, 2011.
3. T. H. Lowry, K. S. Richardson, Mechanism and Theory in Organic Chemistry, 2nd edition, Harper and Row Publishers, New York, 2013.

CY6207: QUANTUM CHEMISTRY, ELECTROCHEMISTRY AND CHEMICAL KINETICS [2 1 0 3]

Quantum Chemistry: Solution of differential equations by power series method, solution of the Schrödinger equation for the hydrogen atom. Electrochemistry: Metal/Electrolyte interface, structure of the double layer, fundamental of electrolytic corrosion. Conversion and Storage of Electrochemical Energy: Fuel cell, efficiency, kinetics, porous electrode, types of fuel cell, batteries, classical of batteries, modern batteries, and electrochemical capacitor for energy storage. Chemical Kinetics: order or reaction, kinetic equivalence terms, theory of reaction rates, elementary gas phase reactions, fast reaction kinetics, chain reactions, acid base catalysis, kinetics in the excited electronic states, physical and chemical adsorption, adsorption isotherms, Langmuir Hinshelwood and Eley Rideal mechanisms, heat of adsorption, kinetics of solid state reactions.

References:

1. N. Levine, Quantum Chemistry, Oxford University Press, 2000.
2. K. J. Laidler, Chemical Kinetics, Harper and Row, New York, 2007.
3. J. O. Bockris, A. K. N. Reddy, Modern Electrochemistry 2B, Kluwer Academic/Plenum Publishers, 2018.
4. M. J. Pilling, P. W. Seakins, Reaction Kinetics, Oxford Univ. Press, 2nd Edition, 2009.
5. J. Rajaram, J. C. Kuriacose, Kinetics and Mechanism of Chemical Transformations, Macmillan India, 2012.
6. D. C. McQuarrie, Quantum Chemistry, Viva Books, 2018.

CY6230: ADVANCED CHEMISTRY LABORATORY-II [0 0 8 4]

Qualitative and Quantitative Analysis: Less common metal ions (two metal ions in cationic/anionic forms), Insoluble – oxides, sulphates, and halides, Separation and determination of two metal ions mixtures using volumetric and gravimetric methods, Chromatography: Separation of cations and anions, Preparations: Preparation of selected inorganic compounds and their studies by spectroscopic methods. Qualitative Analysis: Separation, purification and identification of the components of mixture of three organic compounds (three solids or two liquids one solid, or two solids one liquid) using TLC for checking the purity of separated compounds, chemical analysis using UV and IR spectral data, Multi-step synthesis of organic compounds, Spectrophotometric (UV-VIS) estimation: Amino acid, Proteins, Carbohydrates, Cholesterol, Ascorbic acid, Aspirin etc.

References:

1. B. S. Furniss et al., Vogel's Textbook of Practical Organic Chemistry, Pearson Education, 2003.
2. G. Svehla, B. Sivasankar, Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012.
3. S. K. Maity, N. K. Ghosh, Physical Chemistry Practical, New Central Book Agency, 2012.
4. A. K. Srivastava, Instrumental Approach to Chemical Analysis, S Chand & Co., 2010.

MA6205: RESEARCH METHODOLOGY & TECHNICAL WRITING [2 1 0 3]

Foundations of Research: Meaning, objectives, motivation, utility, empiricism, deductive and inductive theory, characteristics of scientific method, understanding the language of research. Research Process: Problem identification & formulation, research question, investigation question, measurement issues, hypothesis, qualities of a good hypothesis, types of hypothesis. Research Design: Concept and importance in research, features of a good research design, exploratory research design, descriptive research designs, experimental research design. Types of Data: Classification of data, uses, advantages, disadvantages, sources. Measurement: Concept of measurement, problems in measurement in research, validity and reliability, levels of measurement. Statistical Techniques and Tools: Introduction of statistics, functions, limitations, graphical representation, measures of central tendency, measure of dispersion, skewness, kurtosis, correlation, regression, tests of significance based on t, F, Chi-square, Z and ANOVA test. Paper Writing: Layout of a research paper, Scopus/Web of Science

journals, impact factor of journals, when and where to publish, ethical issues related to publishing, plagiarism and self-plagiarism, Introduction to LATEX and MATLAB.

References:

1. C. R. Kothari, Research Methodology Methods & Techniques, New Age International Publishers, Reprint 2008.
2. R. Singh, Research Methodology, Saga Publication, 2014.
3. R. Pratap, Getting Started with MATLAB, Oxford University Press, 2010.
4. S. Kottwitz, LaTeX beginner's Guide, Packt Publications, 2010.
5. J. Anderson and M. Poole, Thesis and Assignment Writing, Wiley, 2011.
6. M. Gupta and D. Gupta, Research Methodology, PHI, 2011.
7. S.C. Gupta and V. K. Kapoor, Fundamentals of Mathematical Statistics, S. Chand & Sons, 1999.

THIRD SEMESTER

CY7101: ORGANOMETALLIC CHEMISTRY [2 1 0 3]

Introduction: Classification of organometallic compounds based on hapticity and polarity of M-C bond. Alkyl and Aryl Complexes of Transition Metals: Synthesis, stability and decomposition pathways. Compounds with Metal-Carbon Multiple Bonds: Alkylidenes, alkylidynes, nucleophilic and electrophilic reactions on the ligands. Transition Metal π-complexes: Transition metal π- complexes with unsaturated organic molecules, CO, alkenes, alkynes, allyl, diene, important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis. Bimetallic and Cluster Complexes: Structure and applications in catalysis. Fluxional Organometallic Compounds: Fluxionality and dynamic equilibria in organometallic compounds. Basic Organometallic Reactions: Ligand substitution, oxidative reactions, Importance of organometallic compounds in biological systems.

References:

1. R. C. Mehrotra and A. Singh, Organometallic Chemistry: A Unified Approach, Wiley-Blackwell, 1991.
2. J. E. Huheey, E. A. Keiter, and R.L. Keiter, Inorganic Chemistry, Principles of Structure and Reactivity, Pearson Education, 2014.
3. F. A. Carey, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, Wiley Interscience, 2014.
4. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Prentice Hall, 2015.

CY7104: PHOTOCHEMISTRY, PERICYCLIC REACTIONS AND HETEROCYCLES [2 1 0 3]

Photochemistry: Photochemical reactions, quantum yield, transfer of excitation energy, actinometry. Determination of Reaction Mechanism: Determination of rate constants of reactions. Photochemistry of Alkenes: Rearrangement of 1,4- and 1,5-dienes. Photochemistry of Carbonyl Compounds: Intramolecular reactions of carbonyl compounds-saturated, intermolecular cyloaddition reactions-dimerisations and oxetane formation. Photochemistry of Aromatic Compounds: Isomerisations, additions and substitutions. Miscellaneous Photochemical Reactions: Photo-Fries reaction of anilides, Photo-Fries rearrangement. Pericyclic Reactions: Classification of pericyclic reactions. Electrocyclic Reactions: Conrotatory and disrotatory motions. Sigmatropic Rearrangements: H-shifts and alkyl-shifts, supra and antarafacial migrations. Heterocyclic: Carbocyclic ring systems.

References:

1. A. Gilbert, J. Baggot, Essentials of Molecular Photochemistry, Blackwell Scientific Publication, 2011.
2. J. Singh, Photochemistry and Pericyclic Reactions, New Age, 2012.
3. R. K. Bansal, Heterocyclic Chemistry, New Age International Private Limited, 2017.
4. N. J. Turro, Molecular Photochemistry, W.A. Benjamin Inc., New York, 2012.
5. A. Cox, T.J. Kemp, Introductory Photochemistry, McGraw Hill, 2014.

CY7107: SOLID STATE CHEMISTRY [2 1 0 3]

Crystal Structure: Crystalline and amorphous solids, methods of characterizing crystal structure - powder x-ray diffraction, electron and neutron diffraction. Preparative Methods: Solid state reaction, chemical precursor method, co-Precipitation, sol-gel, metathesis. Methods of Single Crystal Growth: Solution growth, Melt Growth-Bridgeman, Czochralski, Kyropoulus, Verneuil. Chemical vapour transport. Characterization: Thermal analysis: TGA, DTA, DSC. Electrical Properties: Band theory of solids -metals and their properties. Magnetic Properties: Dia, para, ferro, ferri, and antiferro magnetic types. Soft and hard magnetic materials. Optical Properties: Luminescence of d- and f- block ions. Structural probes. Up and down conversion materials. Superconductivity: Basics, discovery and high Tc materials. Additional Topics: Amorphous materials, zeolites, fullerenes and nanocrystalline solids.

References:

1. A. R. West, Solid State Chemistry and its Applications, John Wiley & Sons, 2007.
2. L. Smart, E. Moore, Solid State Chemistry - An Introduction, Chapman & Hall, 2012.
3. H. V. Keer, Principles of the Solid State, Wiley Eastern Limited, 2013.
4. D. K. Chakrabarty, Solid State Chemistry, New Age Publishers, 2013.

CY7130: ADVANCED CHEMISTRY LABORATORY-III [0 0 6 3]

Spectrophotometric Determination: Manganese/Chromium/Vanadium in steel sample, Fluoride/Nitrite/Phosphate, Zirconium-Alizarin, Red-S Complex Mole – ratio method, Copper-Ethylene diamine complex Slope – ratio method, Flame-photometer Determinations: Sodium and potassium when present together, Lithium/calcium/barium/strontium, Sulphate, Phosphate, Silver. Thermodynamics: Determination of partial molar volume of solute (KCl) and solvent in a binary mixture, Determination of temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO-water mixture) and calculate the partial molar heat, Spectroscopy: Determination of pKa value, Determination of stoichiometry and solubility constant of inorganic and organic complexes, Characterization of the complexes by electronic and IR spectral data,

References:

1. B. S. Furniss et al., Vogel's Textbook of Practical Organic Chemistry, Pearson Education, 2003.
2. G. Svehla, B. Sivasankar, Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012.
3. S. K. Maity, N. K. Ghosh, Physical Chemistry Practical, New Central Book Agency, 2012.
4. A. K. Srivastava, Instrumental Approach to Chemical Analysis, S Chand & Co., 2010.

DISCIPLINE SPECIFIC ELECTIVES (DSE)

DSE – I [Group A (Inorganic)]

CY7140: PHOTO INORGANIC CHEMISTRY [2 1 0 3]

Principles of Photochemistry: Absorption, excitation, photochemical laws, quantum yield. Photochemical Properties of Transition Metal Complexes: Photo physical process, Photochemical process, Photo substitution reactions, photoredox reactions, Photorearrangement reaction, Prompt and Delayed Photochemical reactions, Photolysis rules and ligand field theory. Charge Transfer Photochemistry: Introduction, charge transfer absorption spectra, types of charge transfer excitations and their energy level scheme for charge transfer excitations, Types of reactions observed by charge transfer metal complexes. Ligand Field Photo chemistry of Transition Metal Complexes: Photochemistry Cr(III) of complexes. Photochemistry of Co(III) complexes: Introduction, energy level diagram, Photo aquations in Co(III) amine, Co(III) cyanide complexes, Fe(II) low spin complexes, Ru(II) ammine derivative complexes. Photochemical Reactions on Solid Surface: Introduction, photo electron transfer mechanism, energy level diagram of solid acceptor and donor levels, Examples of photo catalytic metal/mixed metal oxides and their applications.

References:

1. A.W. Adamson, and P.D Fleischauer, Concepts of Inorganic Photochemistry, Wiley, New York, 2007.
2. A. B. P Lever, Inorganic Electronic Spectroscopy, Elsevier Science. London, 2008
3. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age International, New Delhi, 2009.

CY7141: BIO-INORGANIC CHEMISTRY [2 1 0 3]

Transition Elements in Biology - their occurrence and function, active-site structure and function of metalloproteins and metalloenzymes with various transition metal ions and ligand systems. O_2 binding properties of heme (haemoglobin and myoglobin) and non-heme proteins hemocynin & hemerythrin), their coordination geometry and electronic structure, co-operativity effect, Hill coefficient and Bohr Effect. Characterization of O_2 bound species by Raman and infrared spectroscopic methods. Representative synthetic models of heme and non-heme systems. Electron Transfer Proteins - active site structure and functions of ferredoxin, rubridoxin and cytochromes, and their comparisons. Vitamin B12 and cytochrome P450 and their mechanisms of action. Metals in Medicine - therapeutic applications of cis-platin, radio-isotopes and MRI agents. Toxicity of Metals: Cd, Hg and Cr toxic effects with specific examples.

References:

1. Bertini, H. B. Gray, S. J. Lippard & J. S. Valentine, Bioinorganic Chemistry, Viva Books Pvt. Ltd., 2004.
2. S. J. Lippard & J. M. Berg, Principles of Bioorganic Chemistry, Panima Publ. Corpn, 2011.
3. E. I. Ochiai. Bioinorganic Chemistry – An Introduction, Allyn and Bacon Inc., 1977.
4. M. N. Hughes. The Inorganic Chemistry of Biological Processes, Wiley, 1981.
5. R. R. Crichton, Biological Inorganic Chemistry: An Introduction, Elsevier, 2008.

CY22142: NUCLEAR AND RADIOCHEMISTRY [2 1 0 3]

Radioactivity: recapitulation: types of radioactive decay, decay kinetics, radiation detection and measurement (G. M. and Scintillation Counter) Elements of Radiation Chemistry: Interaction of ionizing radiation with matter, units for measuring radiation absorption and radiation energy, radiation dosimetry, radiolysis of water and aqueous solutions. Applications of Radioisotopes - General principles of using radioisotopes, applications of radiotracers in: (1) Physicochemical constants - diffusion coefficient, surface area, solubility, stability constant. (2) Chemical pathways - kinetic studies, inorganic reactions, organic reaction, biosynthesis, polymerization. (3) Trace analysis of elements and compounds - neutron activation analysis, isotope dilution analysis.

References:

1. H. J. Arnikar, Essentials of Nuclear Chemistry, 4th Edition Wiley Eastern, 2007.

2. H. J. M. Bowen, Chemical Applications of Radioisotopes, Buttler and Tanner 2007.
3. G Friedlander, T. W. Kennedy, E. S. Macias and J. M. Miller, Introduction of Nuclear and Radiochemistry, 3rd Edition, John Wiley, 2008.

CY7143: METALLURGICAL SCIENCE [2 1 0 3]

Introduction to Material Science of Metallurgy: Classification, requirements, structure properties-performance correlationship. introduction to levels of internal structure, methods/tools to reveal the different levels of structure, crystal geometry and crystal imperfections, unit cell, crystal structure, Bravais lattice, atomic packing, coordination number, crystal structures of metallic elements, crystal directions and planes, Miller indices, polymorphism, Crystal structure and Correlated Properties: diffusion processes, crystallization – mechanism, factors influencing nucleation and growth, imperfections in crystals and their effect on properties, Solute strengthening. Plastic Deformation: Slip, twinning, strain hardening – mechanism and effect on properties, recovery, recrystallization and grain growth and their effect on properties of ductile metals.

References:

1. R. Balasubramaniam, Callister's Material Science and Engineering, Wiley India, 2009.
2. H. Lawrence Van Vlack Elements of Material Science and Engineerin, Pearson Education, 2012.

DSE – II [Group B (Organic)]

CY7150: MEDICINAL CHEMISTRY [2 1 0 3]

Classification and Nomenclature of Drugs: Synthesis and application. Antibiotics: Synthesis of Streptomycin, penicillins, cephalosporin-C, chloroamphenicol, tetramycin. Antidiabetics: Synthesis of Sequence of A-and B-chains of insulin, glibenclamide, metformin, ciglitazone. Antihistamines: Synthesis of Methapyrilene, chlorpheniramine. Antivirals: Synthesis of Acyclovir, amantidine, rimantidine and Zidovudine. Antineoplastic Agents: Synthesis of mechlorethamine, cyclophosphamide, melaphan, uracil mustards and 6-mercaptopurine. Cardiovascular Drugs: Synthesis of amyl nitrite, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol and oxrprenol. Local Anti-infective Agents: Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, dapsone, aminosalicylic acid, isoniazide, ethionamide, ethambutal, fluconazole, econozole, griseofulvin. Psychoactive Drugs: Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium, gluethimide.

References:

1. G. R. Chatwal, Synthetic drugs, Himalaya, New Delhi 2005.
2. W. D. Foye, T. L. Lemke, D. A. Williams, Principles of Medicinal Chemistry 4th Edition, Wiley India, New Delhi, 2009.
3. R. B. Siwerman, Organic Chemistry of Drug action and Design, Academic press, New Delhi, 2010.

CY7151: CHEMISTRY OF BIOMOLECULES [2 1 0 3]

Cell Structure: Chemistry of biomolecules basic aspects of structure and classification of carbohydrates, lipids, amino acids, proteins and nucleic acids. Supramolecular Assemblies: biomembranes, lipo and glycoproteins. Biocatalysis: thermodynamic and kinetic considerations, concept of enzyme catalysis, role of vitamins and metals as cofactors, enzyme kinetics, Michelis Menten equation. Inhibition of enzyme action, regulatory aspects. Metabolism: Overview and important relationships between glycolysis, TCA cycle, HMP shunt, oxidation of fatty acids, amino acids and urea cycle. Bioenergetics: thermodynamic considerations, redox potentials, bioenergetic principles, mitochondrial electron transport, oxidative phosphorylation process, ATP synthetase, photophosphorylation. Flow of Genetic Information: nature of genetic code, replication of DNA, transcription and translation, regulation of gene expression.

References:

1. A. L. Lehninger, David L. Nelson, Michael M. Cox. Principles of Biochemistry, CBS Publishers, 2010.
2. L. Stryer, Biochemistry, W.H. Freeman and Company, 2012.

CY7152: BIO-ORGANIC CHEMISTRY [2 1 0 3]

Amino acids: Peptides-naturally occurring peptides, modern methods of peptide synthesis with protection and deprotection, proteins, primary, secondary, tertiary and quaternary structure, Enzyme active sites, allosteric sites, and mechanism of their actions e.g. chymotrypsin, carboxypeptidase, lipases. Lipids: Introduction, classification and biological importance of fatty acids and lipids, chemical synthesis of phospholipids and glycolipids. Structure, Physical and Chemical Properties: Heterocyclic bases-adenine, guanine, cytosine, uracil and thiamine, chemical and enzymatic hydrolysis of nucleic acid, structure and function of DNA, RNA (m-RNA, t-RNA, r-RNA).

References:

1. A. L. Lehninger, David L. Nelson, Michael M. Cox. Principles of Biochemistry, CBS Publishers, 2010.
2. L. Stryer, Biochemistry, W.H. Freeman and Company, 2012.

CY7153: TEXTILE CHEMISTRY [2 1 0 3]

Introduction: Classification of textile fibres according to their nature and origin. Natural Fibres: Vegetable (leaf and seed fibres), animals (wool and silk) and c) mineral (glass, asbestos and metallic fibres). Man-made Fibres: Classification, regenerated fibres-acetate, viscose, Synthetic Fibres: principles of polycondensation with reference

to polyesters, polyamides and polyurethanes. Texturing: Introduction, purpose, bulked and textured yarns, methods of texturing thermoplastic and non-thermoplastic yarns, basic principles.

References:

1. R. W. Moncrieff, Manmade Fibres, Wiley, New York, 2005.
2. E. R., Trotman, E. R., Dyeing and Chemical Technology of Textile Fibres, Lubrecht & Cramer Ltd, Port Jervis, 2011.
3. M. Lewin, Handbook of Fiber Chemistry, 3 rd Edition, CRC Press, 2012.

DSE – III [Group C (Physical)]

CY7160: COMPUTATIONAL CHEMISTRY [2 1 0 3]

Fundamentals of Computational Chemistry: Component of computer system, computer language, PC, an introduction to Disk Operation System (DOS) and Windows. Computer Applications: Application package for report generation and presentation, MS-office- introduction to MS-word, document and manipulations, saving and printing, incorporation of graphs, tables, pictures and chemical structures into the document. Excel: spreadsheets, report generation, data base management, and graphical representation of tabulated data. Elements of Computer Architecture: Evaluation of analytical wave functions and graphing, 3D and contour plots, Regression analysis of experimental data, linear and non-linear deconvolution techniques. Computer Applications in Chemistry: Development of small computer codes involving simple formulae in chemistry, such as van der Waals equation, pH titration, kinetics, radioactive decay, Evaluation of lattice energy.

References:

1. P. C. Jurs, Computer software applications in chemistry, Wiley India, New Delhi, 2009.
2. K. J. Johnson, Numerical Methods in Chemistry, Marcel Dekker, New Delhi, 2010.
3. A. F. Carley, and P. H. Morgan, Computational Methods in the Chemical Science, Eillis Horwood Ltd, New York, 2011.

CY7161: BIOPHYSICAL CHEMISTRY [2 1 0 3]

Chemistry and Biology: Amino acids, proteins, enzymes, DNA & RNA in living systems, electrolytes, the chirality of biological molecules. Physical Aspects of Biopolymers: X-ray diffraction, electronic absorption & luminescence Spectroscopy, optical activity, magnetic activity, magnetic-optical activity. Photo Biological Processes: Photosynthesis, mechanism of vision, the molecular mechanism of photoreceptor. Mechanochemical Processes: Introduction, thermodynamics, nerve conduction and membrane equilibria, muscle and muscle proteins, their chemistry and physics.

References:

1. K. Upadhyay, N. Upadhyay, N. Nath, Biophysical Chemistry, Himalaya Publishing House Pvt. Ltd., 2016.
2. J. B. Davidson, D. V. Hobbs, J. B. Harborne, R.S. Mann, Natural Products: Chemistry & Biological Significance Longmar Essex, 2007.
3. D. L. Nelson, M. M. Cox, Lehninger's Principles of Biochemistry, W. H. Freeman, 2015.
4. Satyanarayana, Biochemistry, Elsevier, 2017.

CY7162: ADVANCED QUANTUM CHEMISTRY [2 1 0 3]

Introduction: Vector Interpretation of Wave function, Hermitian Operator, The Generalized Uncertainty principle, The quantum Mechanical Virial Theorem, Solution of harmonic oscillator (Operator approach), Second quantization (Boson and Fermion). Approximate solutions to the Schroedinger equation: The Variation method (Time independent and Time Dependent), Time independent perturbation theory. The Antisymmetry Principle, Spin angular momenta and their Operators, The Orbital Approximation. The Hartree-Fock Self-Consistent Field Method: The generation of Optimized orbitals, Koopman's Theorem (The Physical Significance of Orbital Energies), The electron correlation energy. Introduction to Molecular Structure: The Born - Oppenheimer Approximation, Solution of the Nuclear Equation. Electronic Structure of Linear Molecules: The MO - LCAO Approximation, The Hydrogen Molecule Ion, The Hydrogen molecule, Molecular Configuration-Interactions.

References:

1. F. L. Pilar, Elementary Quantum Chemistry, McGraw Hill Publishing Company, 2012.
2. P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, Oxford Univ. Press, 2013.

CY7163: LIQUID STATE [2 1 0 3]

Liquid State: Properties of liquids: Surface tension (γ), viscosity and their relationship to chemical constitution. Glassy state (Amorphous solids): Glass: Manufacture of glass: Types of Glasses. Liquid Crystals: Mesomorphic state, examples that exhibit mesomorphic state. Vapour pressure – Temperature curves for mesomorphic substances – classification of liquid crystals – smectic. Nematic. and cholesteric liquid crystals and examples. Principle of liquidcrystal displays (LCD's), Discotic liquid crystals. polymer liquid crystals – Molecular arrangement in various types of liquid crystals.

References:

1. S. Glasstone and D. Lewis, Essentials of Physical Chemistry. Prentice Hall India, 2010.
2. K.L. Kapoor, Physical Chemistry, S. Chand and Co. New Delhi, 2012.

3. W. Skoog, W. Holler & Crouch, Fundamentals of Analytical Chemistry, Wiley, 2013.

CY7164: CATALYSIS TECHNOLOGY [2 1 0 3]

Introduction to Heterogeneous Catalytic Processes: Adsorption on solid surfaces , Solid catalyst: types, formulations and preparation methods, various catalysts characterization methods: catalysts testing and types of reactors, Effect of external and internal transport processes on reactions rate, Mechanism and Kinetics Study: Kinetic modeling and Parameter estimations, Catalyst deactivations, Industrial catalytic processes , New development in solid catalysis, nano catalysts, monoliths, environmental catalysts, fuel cell catalysts, Design of catalysis, simulation techniques.

References:

1. G. Ertl, H. Knozinger, and J. Weitkamp, Handbook of Heterogeneous Catalysis, Wiley – VCH, 2011.
2. B. Viswanathan, S. Sivasanker, A. V. Ramaswamy, Catalysis: Principles & Applications, CRC Press, 2014.