Semester – I			
Core I	**Inorganic Chemistry - I**		
Code : 19PCHC11	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Vision:

To impart the students with basic principles and concepts in chemistry.

Mission:

- To understand the atomic structure and periodical properties of elements.
- To explain the various concepts of acids and bases.
- To know the basics of organometallic chemistry.
- To demonstrate the principle and applications of IR, Raman and Mossbauer spectroscopies.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO - 1	explain about the electronic configuration, orbital stability and the reactivity	1,3	Ap
CO - 2	discuss the periodic properties of the elements	1,7	An
CO - 3	demonstrate the theories of VSEPR, Valance bond and Molecular Orbital.	1,8	Ap
CO - 4	point out Arrhenius, Bronsted - Lowry and Lewis theories of acids and bases.	2,3	Cr
CO - 5	compare the chemistry of Non-aqueous solvents such as liquid ammonia, Liquid hydrogen fluoride, Liquid Sulfur dioxide .	1,3	An
CO - 6	synthesis and discuss reactivity of metal alkyls, carbenes, carbynes, carbides, alkenes, alkynes, and arene complexes	2,3	Cr
CO - 7	predict the number of active modes of vibrations in IR and Raman spectroscopy.	2,6	Un
CO - 8	interpret the Mossbauer spectra of Iron and Tin complexes.	2,5	Ev

Semester – I			
Core I	**Inorganic Chemistry - I**		
Code : 19PCHC11	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Unit I Periodic properties and Ionic Bonding

Periodic properties of elements - Ionic radii, ionization potential, electron affinity, electronegativity, Bond lengths, bond strength, bond angles, bond order, bond energies andlattice energy.

Chemical bonding - Ionic Bond - Properties of ionic substances - Lattice energy - Born-Haber cycle - Size effect: Ionic Radii - Factors affecting radii of ions - Covalent character predominantly in ionic bonds - Polarization - Fajan's rule - Results of polarization. Oxidation reduction reactions - The use of Reduction potentials to predict: Oxidising reducing species, Stability and elements having several oxidation states.

Unit II Molecular structure and Bonding

Lewis electron dot diagrams - Hybridization, Octet rule - Resonance VSEPR theory - Walsh diagram (H_2O) - Bent's rule – Apicophilicity - Valence bond theory - MO theory of homo and heteronuclear diatomic molecules and poly atomic molecules (O_2, N_2, CO, HCl and $BeCl_2$) - Geometrical isomerism - Fluxionality - Types of chemical bonds (weak and strong) - Intermolecular forces.

Unit III Acids and Bases

Acid-base theories - Arrhenius, Bronsted- Lowry theory, Factors affecting strength of acids and bases - Lewis theory - Catalytic behavior of acids and bases - The Hard soft interaction principle (HSIP), Proton affinity.

Non-aqueous solvents - Chemistry in liquid ammonia, liquid hydrogen fluoride, liquid sulfur dioxide - Super acids.

Unit IV Organometallic chemistry I

16 and 18 electron rules, synthesis, structure and bonding in mono and polynuclear metal carbonyls, carbonylate ions, carbonyl hydride complexes - Isolobal fragments - Synthesis and reactivity of metal alkyls, carbenes, carbynes, carbides, alkenes, alkynes, and arene complexes - Metallocenes and bonding in metallocenes.

Unit V Spectroscopy I

IR and Raman: Selection rules - Predicting number of active modes of vibrations - Applications of IR and Raman in the study of inorganic structures and coordination compounds - Application of isotopic substitution, detection of intra and intermolecular hydrogen bonding.

Mossbauer: Principle, conditions for Mossbauer spectroscopy - Isomer shift - Quadrupole interactions - Magnetic interactions - Interpretation of spectra of iron ($Na_2Fe(CN)_6$, $Fe(CO)_5$, $Fe_2(CO)_9$) and tin ($(C_6H_5)_3SnX$) compounds.

Text Books:

1. James E.Huheey, Ellen.A. Keiter and Richard .L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, Harper Collins College Publishers, 4th Edition, 1993.
2. Skoog D.A, West D.M, Holler F.J, Grouch S.R., Fundamentals of Analytical Chemistry, Thomson Asia Pvt. Ltd., Eighth Edition, Third Reprint, 2005.
3. Shriver D.F., Atkins P.W. and Langford C.H., Inorganic chemistry, ELBS, Oxford University Press, 1994.

Books for Reference:

1. Lee J.D., Concise Inorganic Chemistry, Blackwell Science Ltd., 5th Edition, 2003.
2. Albert Cotton F., Geoffrey Wilkinson, Carlos. A.Manic and Manfred Bochman, Advanced Inorganic Chemistry, Wiley Interscience Publication, 6th Edition, 1999.
3. James E. House Inorganic chemistry, Elsevier Publications, 2008.
4. Purcell K.F. and Kotz J.C, Inorganic Chemistry, WB Saunders Company, Philadelphia, 1977.
5. Drago R.S., Physical Methods in Inorganic Chemistry, WB Saunders Company, 3rd Edition, 1977.
6. Ebsworth David E.A.V., Rankin Stephen Credock W.H., Structural Methods in Inorganic Chemistry, ELBS, IV, 1988.

Semester – I			
Core III	**Physical Chemistry - I**		
Code : 19PCHC13	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Vision

To achieve base knowledge about the concepts of physical chemistry.

Mission

- To solve Schrodinger equations for a particle moving in different dimensions.
- To demonstrate and prepare the polymer molecules by various methods.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO - 1	have a good foundation in understanding the physical and mathematical aspects of quantum mechanics.	1	Un
CO - 2	know the limitations of quantum chemistry and classical thermodynamics in the evaluation of macroscopic properties.	4	An
CO - 3	apply the approximation methods to different atoms and find the dissociation energy and bond order for various molecules by applying Huckel molecular orbital theory.	7	Ap
CO - 4	discuss in detail about partial molar properties.	1	Ap
CO - 5	explain different types of methods of preparation of polymers.	6	Un
CO - 6	prepare the polymer molecule and determine the molecular weight of polymer.	6	Cr
CO - 7	classify the molecules according to their moment of inertia.	1	An
CO - 8	explain the fundamentals of molecular spectroscopy.	4	Un

Semester – I			
Core III	**Physical Chemistry - I**		
Code : 19PCHC13	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Unit I Quantum Chemistry – I

Limitations of classical mechanics – Schrodinger equation - Postulates of quantum mechanics - Operators and their algebra - linear operator, Hermitian operators - Eigen functions and Eigen values - Schrodinger equations (Time dependent and Time independent) – Particle in a box (1D and 3D) - Hydrogen atom - Rigid rotor and simple harmonic oscillator - Quantum mechanical tunneling.

Unit II Quantum Chemistry – II

Pauli exclusion principle - Slater determinant – Approximation methods - Variation theorem - Application of variation method to helium atom - Perturbation theory (First order) - Application to helium atom - Hartree Fock Self consistent field method (HF-SCF) to helium atom - Born-Oppenheimer approximations – MO and VB treatments of H_2^+ molecular ion and H_2 molecule - Huckel Molecular Orbital theory - Application to ethylene, butadiene and benzene.

Unit III Thermodynamics

Concepts of partial molar properties – Partial molar free energy, chemical potential, partial molar volume and its significance - Gibbs-Duhem equation - Gibbs-Duhem-Margulus equation - Determination of partial molar volume - Graphical method, intercept method and apparent molar volume method. Concept of fugacity - Determination of fugacity by graphical method and compressibility factor method - Concept of Activity and activity coefficient -Determination of activity and activity coefficients for non-electrolytes.

Unit IV Polymer Chemistry

Polymerization in homogeneous and heterogeneous phases – Kinetics and mechanism of addition polymerization (Free radical and cationic) and condensation – Kinetics of copolymerization – Molecular weights – Distribution and methods of determination - light scattering, ultracentrifuge, viscosity, osmometry and gel permeation chromatography. Conducting polymers - Factors affecting the conductivity of conducting polymers - Doping of conducting polymers - solitons , polarons and bipolarons.

Unit V Rotational Spectroscopy

Electromagnetic radiation - Quantization of energy - rotational, vibrational, and electronic energy levels and transitions in molecules - Regions and representation of spectra – Width of spectral lines - Collision broadening, Doppler broadening, Heisenberg uncertainty principle - Intensity of spectral lines - Transition probability - Diatomic molecules as rigid rotors
- Rotational energy levels, intensity of spectral lines, selection rules - Effect of isotopic

substitution - Diatomic molecules as non-rigid rotors - Rotational transitions - Rotational spectraof linear and symmetric top polyatomic molecules.

Text Books:

1. A. K. Chandra, Introductory Quantum Chemistry; 4th Ed., Tata McGraw Hill, Noida, 1994.
2. Aruldhas.G., Quantum Mechanics, Prentice Hall of Indian Pvt. Ltd, , New Delhi, 2006.
3. R. K. Prasad, Quantum Chemistry, 4th Ed., New Age International Publishers, New Delhi,2014.
4. K. Rajaram and J.C. Kuriacose, Thermodynamics for Students of Chemistry, 2nd Edition, S.L.N. Chand and Co, Jalandhar, 1986.
5. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 4th Ed., McGraw Hill Education,Noida, 1994.

Books for Reference:

1. D. A. Mcquarrie, Quantum Chemistry, University Science Books, Sausalito, 2008.
2. I. N. Levine, Quantum Chemistry, 5th Ed., Prentice Hall, New Jersey, 2000.
3. Atkins P W, Molecular Quantum Mechanics, Clarendon, 1973.
4. Anatharaman R, Fundamentals of Quantum Chemistry, McMillan, NewDelhi, 2001.
5. I. N. Levine, Quantum Chemistry, Prentice Hall India, 1994.
6. Moore.W.J, Physical chemistry, Prentice-Hall of India Pvt. Ltd. 1962.
7. Atkins.P.W - Physical chemistry, ELBS edition of third edition, 1987.
8. M. Ladd, Introduction to Physical Chemistry, Cambridge, 1998.
9. S.H. Maron and J.B. Lando, Fundamentals of Physical chemistry, MacMillan Publishers,New York, 1974.
10. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry - Classical,Statistical and Irreversible, Pearson Education, New Delhi, 2013.
11. I.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, 6th Edition, W.A. BenjaminPublishers, California, 1972.
12. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1964.

Semester – II			
Core IV	**Inorganic Chemistry - II**		
Code : 19PCHC21	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Vision:

To promote the advance knowledge about complexes and spectroscopy**.**

Mission:

- To discuss the stability and bonding in Co-ordination compounds.
- To understand the chemistry of inner transition elements.
- To explain the principle and applications of photoelectron and auger spectroscopy.

Course outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO - 1	judge about the stability and factors affecting the stability of the coordination complexes.	1,2	Ev
CO – 2	catagorise the ligands into strong and weak by Irving William series and the spectrochemical series.	2,3	An
CO - 3	discuss the various features of Valence bond, Crystal field and Molecular orbital theories.	1,7	An
CO - 4	measure Crystal Field Stabilisation Energy (CFSE) (10Dq or Δ_0) of coordination complexes.	4	Ev
CO - 5	summarise the substitution, oxidative addition, reductive elimination, nucleophilic and electrophilic reactions of organometallic complexes.	2,3	Un
CO - 6	compare the properties of elements present in Lanthanides and Actinides.	1,5	An
CO - 7	calculate the Microstates and Term symbols for Transition metal complex.	4,8	Ev
CO - 8	discuss the applications of XPES and UVPES to inorganic spectra.	5,6	An

Semester – II			
Core IV	**Inorganic Chemistry - II**		
Code : 19PCHC21	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Unit I Stability of Co-Ordination compounds

Coordination numbers and structures, isomerism- Stability constants of complexes and their determination – Solubility method, Ion exchange method, Job's method and Bjerrum's method –Stabilisation of Unusual oxidation state - Irving William series and the spectrochemical series – Factors affecting stability constant - Chelate and Macrocyclic effect.

Unit II Bonding in Co-ordination compounds

Valence bond theory - Crystal field theory – Crystal Field Stabilisation Energy (CFSE) – Measurement of 10Dq or Δ_0 – Determination of factors affecting magnitude of Δ_0 or 10Dq: geometry of the complex, oxidation state of the central metal ion, principal quantum number of the d-orbital and nature of ligands – Consequences of crystal field splitting: ionic radii of transition metal ions, hydration energy, lattice energy, unusual oxidation states and CFSEs - Spinels and inverse spinels – Jahn-Teller effect - Molecular orbital theory (sigma as well as Pi bonding).

Unit III Organometallic chemistry II

Reactions of organometallic complexes - Substitution, oxidative addition, reductive elimination, nucleophilic and electrophilic displacement of coordinated ligands, Homogeneous Catalysis - Hydrogenation, Hydroformylation, Monsanto process, Wacker process, Alkene metathesis, heterogeneous catalysis - Fischer-Tropsch process, Ziegler-Natta polymerization.

Unit IV Lanthanides and Actinides

Occurrence, properties of the elements - Common and uncommon oxidation states - Absorption and emission Spectra - magnetic properties - Separation of lanthanide elements - lanthanide and actinide contraction - similarities between actinides and lanthanides -Coordination complexes and Organometallic compounds of lanthanides and actinides - Uses of lanthanide compounds as shift reagents.

Unit V Spectroscopy II

Electronic spectroscopy - Microstates, Term symbols, selection rules - Orgel and Tanabe-Sugano diagrams - Charge transfer spectra - Electronic spectra for 1^{st} row transition metal complexes - Calculation of Dq, B for octahedral d^2 and d^8 systems - Nephelauxetic ratio - Electronic spectra of lanthanide and actinide.

Photo electron spectroscopy – UVPES - Principle, spin-orbit coupling – XPES – Principle, chemical shift in XPES - Koopman's theorem - Applications of XPES and UVPES to inorganic spectra - Auger electron spectroscopy

Text Books:

1. James.E.Huheey, Ellen.A.Keiter and Richard.L.Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, Harper Collins College Publishers, 4th Edition,1993.
2. Shriver D.F., Atkins P.W. and Langford C.H., Inorganic chemistry, ELBS, Oxford University Press, 1994.
3. R.Gopalan, Textbook of Inorganic chemistry, Universities Press (India) Private Limited, 2012.
4. Skoog D.A, West D.M, Holler F.J, Grouch S.R., Fundamentals of Analytical Chemistry, Thomson Asia Pvt. Ltd., Eighth Edition, Third Reprint, 2005.

Books for Reference:

1. Robert H. Crabtree The Organometallic Chemistry of the Transition Metals, John Wiley& Sons, Inc., Publication, 4th Edn, 2014.
2. Gary L. Miessler, Donald A. Tarr, Inorganic chemistry. Pearson Publications, 5th edition,2014.
3. Catherine Housecroft, Alan G. Sharpe, Inorganic Chemistry, 3rd Edition, Prentice Hall,2007.
4. Albert Cotton F., Geoffrey Wilkinson, Carlos .A.Manic and Manfred Bochman, Advanced Inorganic Chemistry, Wiley Interscience Publication, 6th Edition , 1999.
5. Purcell K.F. and Kotz J.C, Inorganic Chemistry, WB Saunders Company, 1977.
6. Bertini I., Gray H.B, Lippard S.J. and Valantine J.S, Bioinorganic Chemistry, Viva Books Pvt. Ltd, 1998.
7. H.H., .Merritt L.L and Dean J.A, Instrumental Methods of Analysis, CBS Publishers, 6thedition, 1986.
8. Frank A. Settle, Handbook of instrumental techniques for analytical chemistry, Prenticehall, 1997
9. Drago R.S., Physical Methods in Inorganic Chemistry, W.B. Saunders Company, 1977.
10. Ebsworth David E.A.V., Rankin Stephen Credock W.H., Structural Methods in InorganicChemistry, ELBS, IV, 1988.

Semester – II			
Core V	**Organic Chemistry - II**		
Code : 19PCHC22	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Vision:

To inspire a knowledge platform that supports an inventive culture. Educate future leaders about how chemistry underlies living systems and physical processes.

Mission:

- To support and advance the worldwide community of chemistry scholars.
- To enhance the basic and applied research framework in the Chemistry Department.
- To understand the principle behind thermal and photochemical organic reactions.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO - 1	organize the various methods of determination of reaction mechanism	6	Cr
CO - 2	comprehend the various factors that operate in organic reactions	3	An
CO - 3	use relevant concepts and terminology in a correct fashion	8	Re
CO - 4	understand the isolation and structural determination of alkaloids	5	Un
CO - 5	determine structure and stereochemistry of Morphine and quercetin	6	Cr
CO - 6	gain knowledge of photochemical organic reactions	5	Ap
CO - 7	discuss the Photochemistry of (n-π^*) transitions with particular reference to Norrish type I , Norrish II type reactions, Paterno Bucchi reactions & photochemistry of nitrites.	8	An
CO - 8	understand the applicability of the spectroscopic techniques	4	Un

Semester – II			
Core V	**Organic Chemistry - II**		
Code : 19PCHC22	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 4**

Unit I Study of Organic Reaction Mechanism

Mechanistic Classification- Thermodynamic requirements for reaction -Kinetic requirements for reactions - Reaction rates- Transition state theory - Hammond Postulate- Microscopic reversibility - Methods of Determining Mechanism: Identification of products, determination of the presence of intermediate, isotopic labelling, Stereochemical evidence, Kinetic evidence, Isotope effects. Reactive intermediates, LFER - Hammett equation – Physical significance of σ and ρ – Applications and Limitations – Taft equation.

Unit II Molecular Rearrangement

Migration of Carbon – Wagner - Meerwein rearrangement, Pinacol-Pinacolone rearrangement, Benzil-Benzilic acid rearrangement and Dienone-Phenol rearrangement. Migration of heteroatoms - Migration to electron deficient nitrogen, Beckmann rearrangement, Curtius rearrangement and Lossen rearrangement.

Migration to electron deficient oxygen – Baeyer-Villiger oxidation, Hydroperoxide rearrangement and Dakin reaction. Migration to electron rich carbon – Neber rearrangement and Tiffenev-Demjanov rearrangement.

Unit III Alkaloids and Flavonoids

Alkaloids – Introduction - General methods of extraction – Classification - Degradation studies - HEM, Emde and Von-Braun - Structural elucidation of papaverine, morphine and quinine, Reserpine.

Flavonoids - Introduction- Properties- Isolation- General methods for the elucidation of structure of flavones, flavonols, Quercetin.

Unit IV Photochemistry Analysis

Photochemical excitation - Experimental techniques; electronic, transitions; Jablonskii diagram; Intersystem crossings; Energy transfer process, Stern-Volmer equation. Reactions of electrically excited ketones; π–π^* triplet; Norrish type I and II cleavage reactions – Photo reductions; Paterno-Buchi reactions, Photochemistry of α, β- unsaturated ketones; cis – trans isomerisation. Photon energy transfer reactions – Photocycloadditions - Photochemistry of aromatic compounds - Barton's reaction and di- π methane rearrangement.

Unit V Ultra Violet – Visible and Infra - Red Spectroscopy

UV – Visible spectroscopy - Absorption laws - Types of electronic transitions – Instrumental and Sampling – Solvent effect – Application of Woodward- Fieser rules for calculating absorption maximum in conjugated diene, triene, polyenes, α and β unsaturated carbonyl compounds.

Optical rotatory dispersion and circular dichroism - Octant rule, α-haloketone rule and their applications.

IR spectroscopy – Basic theory and Instrumentation - Characteristics of IR absorption ofdifferent functional groups - Factors influencing vibrational frequencies – Applications of Infra- red spectroscopy - Identification of Organic compound, Structure determination, Qualitative analysis of functional groups, Distinction between two types of hydrogen bonding, Quantitative analysis, study of a chemical reaction, study of Keto-enol tautomerism, Complex molecules, Conformational analysis, Geometrical isomerism, Rotational isomerism, Detection of impurity ina compound.

Text Books:

1. Kalsi P S,Organic Reaction & Mechanism, 4th Edition,New-Age International Publishers,New Delhi, 2011.
2. Ahluwalia V.K and Parshar R.K, Organic Reaction Mechanism Fourth Edition , NarosaPublishing House, 2013.
3. Mukherjee K.S, Mechanism of Organic reactions, Books and Allied Ltd, Kolkota, 2010.
4. Raj K Bansal, Organic reaction mechanism, 4th edition, New Age international publishers,New Delhi, 2012.
5. Gurdeep Chatwal, Organic Chemistry of Natural Products, Vol II, Himalaya PublishingHouse, Bombay, 2003.
6. Sharma Y.R, Elementry Organic spectroscopy, S.Chand & Company, New Delhi, 2011.
7. Jag Mohan, Organic spectroscopy Principles and Applications, Narosa Publishing House,New Delhi. Second Edition, 2011.

Books for Reference:

1. March J, Advanced Organic Chemistry, Fourth Edition, John-Wiley and Sons, New York,1992.
2. Clayden, Greeves, Warren and Wothers, Organic Chemistry, Oxford University Press,New York, 2006.
3. Finar I L, Organic Chemistry Volume I and II, Sixth Edition, ELBS with Longmann,Singapore, 1997.
4. Sykes P, Guide Book to Mechanism in Organic Chemistry, Sixth Edition, ELBS withLongmann, 1997.
5. Norman R.O.C, J.M. Coxon, Principles of Organic synthesis, Third edition,Chapman and Hall, 1994.

Semester – II			
Core VI	**Physical Chemistry- II**		
Code : 19PCHC23	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Vision

To synthesise the nanomaterials by eco-friendly methods, characterise the synthesized nanomaterials and apply in different fields for the welfare of society.

Mission

To introduce and give an insight into the fascinating area of Nanoscience.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO - 1	recall a thorough knowledge of basics of nanoscience and nanotechnology	4	Re
CO - 2	explain the preparation, characterization and properties of nanomaterials	6	Un
CO - 3	analyze the types and properties of carbon nanotubes	1	An
CO - 4	assimilate existing and new concepts, methodology and researches and apply them in their academic research environment	7	Ev
CO - 5	aware of challenges, risks and promises of nano technological development	6	Cr
CO - 6	synthesise the nanomaterials by physical, chemical and biological methods.	6	Cr
CO - 7	characterise the synthesized nanomaterials by various techniques.	5	Ev
CO - 8	apply the nanomaterials in energy storage, food and in day-to-day life.	8	Ap

Semester – II			
Core VI	**Physical Chemistry- II**		
Code : 19PCHC23	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Unit I Introduction

Definition – Nanoscience and Nanochemistry - Four generations of Nanotechnology development - Definitions of Nanotechnology – Nanostructures (Nanoparticles, Nano scale in one dimension, two dimension and three dimension) - Classification of nanoparticles - Properties of nanomaterials – Surface property, Physico-chemical, Electrical and electronic, Redox, Optical, Mechanical and Magnetic properties.

Unit II Synthesis and characterisation

Synthesis of nanomaterials - Top down and Bottom up approach - Physical methods (Laser Ablation, Evaporation, Sputtering and Gas condensation) - Chemical methods (Thermolysis, Sonochemical approach and Sol-gel synthesis) - Biosynthesis (Elementary idea only) - Structural characterisation of nanomaterials - X-ray diffraction, Scanning Tunneling Microscopy and Atomic force microscopy.

Unit III Carbon nanotube

Carbon nanotube - Carbon allotropes (Diamond ,Graphite, Carbon nanotubes) - Types of Carbon nanotubes - Synthesis of carbon nanotubes - Electric arc Discharge method, Laser method, Chemical vapour deposition method (CVD) - Purification methods, properties andapplications of Carbon nanotubes – Fullerenes - Synthesis and purification - Properties and applications of Fullerenes.

Unit IV Nanocomposites

Definition – Ceramic-matrix nanocomposites – Nanocomposites by mechanical alloying – Metal-matrix nanocomposites – Poymer nanomaterials – Synthesis methods - Solution intercalation – Melt intercalation – Emulsion polymerization – In-situ polymerization – Properties of polymer nanostructured materials – Material properties – Thermoplastic nanocomposites – Nylon 6 nanocomposites – Thermoset nanocomposites – Epoxy nanocomposites – Elastomer nanocomposites – TPO nanocomposites.

Unit V Applications of Nanotechnology

Chemistry and Environment – Water purification - Energy storage - Rechargeable batteries, Hydrogen storage - Information and Communication - Heavy industry - Consumer goods (food, textiles and cosmetics) - Nano medicine - medical applications of molecularnanotechnology (Nanorobots, Cell repair machines, nanonephrology).

Text Books:

1. Khanna.O P, A Text Book of Nanochemistry, Astha Publishers & Distributors,New Delhi, 2014.
2. Shanmugam S, Nanotechnology, MJP Publishers, Chennai, 2011.

Books for Reference:

1. Parthasarathy. B.K, Nanostructure and Nanomaterials, Isha Books, Delhi, 2007.
2. Uday Kumar, Concepts in Nanochemistry, Anmol Publications Pvt. Ltd,New Delhi, 2013.
3. Bandyopadhyay A K, Nano Materials, New Age International Publishers, 2nd Edn, 2012.
4. Viswanathan B, Nano Materials, Narosa Publishing House, New Delhi, 2013.
5. Guozhong Cao, Nanostructures & Nanomaterials - Synthesis, Properties & Applications,Imperial College Press, 2004.

Semester – I			
Elective I A	**Denova Designs In Chemistry**		
Code : 19PCHE11	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Vision:

To develop better predictability of human pathophysiology and biological pathways underlying specific diseases and train the students to innovate new medicines.

Mission:

- To understand about molecular modelling and drug designing.
- To have depth knowledge about host-guest molecules.
- To create awareness about common diseases and their treatments.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO - 1	formulate molecular dynamics in drug design.	5	Ap
CO - 2	perform docking using Autodock virtual screening and De nova designs.	6,8	Cr
CO - 3	develop recent trends in the synthesis of crown ethers.	6	Cr
CO - 4	design a green method for the synthesis of compounds using twelve principles of Green chemistry.	5,6	Cr
CO - 5	organise C++ programming for the determination of some Chemical properties.	8	An
CO - 6	calculate the delocalisation energy for aromatic system.	4	Ev
CO - 7	acquire knowledge about common diseases due to insects, animals, air and water borne diseases.	1,8	Un
CO - 8	compare different dosage forms of drugs such as solid, semisolid, liquid and gaseous dosage form.	8	An

Semester – I			
Elective I A	**Denova Designs in Chemistry**		
Code : 19PCHE11	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Unit I Molecular modelling and Drug designing

Introduction to Molecular modelling - Drug discovery: the Evolution and process - The role of Computer assisted drug design- the process of drug discovery- Bioassay- Lipinski's rule of five. Quantum mechanical simulations - *Ab Initio* methods, Semi Empirical methods- Molecular dynamics in drug design. Docking- types of searching methods in Docking, docking methods, the scoring function, docking using Auto Dock, Virtual screening, De novo design. Cheminformatics - SMILES (Simplified Molecular Input Line Entry Specification) - Applications of Cheminformatics in Drug discovery.

Unit II Supramolecular chemistry

Introduction - Development, Classification - Based on cavity, Based on forces - Recent developments in Supramolecular compounds - Molecular self assembly - Self replicating molecular systems - Molecular self assembly based on hydrogen bond - Metal coordinated self assembly - Catenenes and Rotaxanes - Recent developments in the synthesis of crown ethers - Synthesis of Cryptands - Metal complexes with Crown ethers and Cryptands.

Unit III Green chemistry

Twelve principles - atom economy - Addition and rearrangement reaction, substitution reaction, elimination reaction - Green solvents - Supercritical CO_2, H_2O, Ionic liquids.
Solid state and non solid state microwave assisted reaction – Stille reaction, Suzuki reaction – Krohnke reaction – Hiyama reaction - Sonogashira reaction.

Unit IV Computational chemistry

Introduction - Character set in C++ - Tokens - Keywords, identifiers and constants, variables, operators (Input/Output) - Cascading - Selection of statements - IF, IF …..ELSE, SWITCH, WHILE, DO…..WHILE, FOR, BREAK, CONTINUE and GOTO - Functions - Arrays - Classes - Pointers - Inheritance.

C++ programming for the determination of electronegativity of an atom - Lattice energy using Born - Lande equation - Normality, Molarity and Molality of solutions - Solubility of sparingly soluble salts - Molecular weights of organic compounds - Calculation of delocalisation energy values for aromatic systems.

Unit V Pharmaceutical Chemistry

Introduction - Drugs for common diseases due to insects & animals, Air borne diseases, Water borne diseases, Respiratory diseases & Diseases of the Nervous system - Pharmaceutical Aids - Preservative, Anti oxidants, Sequestrants - Colouring agents, Flavouring agents and

artificial sweetening agents added in drugs. Different dosage forms of Drugs - Solid (Tablet),Semisolid (Paste, Cream), Liquid (Solution, Suspension, Emulsion), Gaseous dosage form.

Text Books:

1. Anand Solomon K, Molecular modelling and Drug Design, MJP publishers, 2016.
2. P.S.Kalsi, J.P.Kalsi, Bioorganic, Bioinorganic and Supramolecular Chemistry, New AgeInternational publishers, Second Edition, 2010.
3. Ramesh Kumari, Computers and their Applications to Chemistry, Narosa PublishingHouse, New Delhi, Second Edition, 2005.
4. K. V. Raman, Computers in Chemistry, Tata McGraw-Hill Publishing Company Limited,New Delhi, Eighth Edition, 2005.

Books for Reference:

1. S.M. Khopkar, Analytical chemistry of Macrocyclic and Supramolecular compounds, Narosa Publishing House, Delhi, Second edition, 2008.
2. Ahluwalia, V. K and Rajender S. Varma, Green Solvents for Organic synthesis, Narosa Publishing House Pvt. Ltd., 2009.
3. Paul T Anastas, Text Book on Green Chemistry, OUP, 2006.
4. Raghupati Mukhopadhyay, Sriparna Datta, Rajib Kumar Das, Textbook of Pharmaceutical chemistry & Medicinal Chemistry, Books and Allied (P) Ltd, First Edition, 2011.

Semester – I			
Elective I B Chemical Instrumentation			
Code : 19PCHE11	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Vision:

To impart the students with basic principles and concepts in Instrumental techniques.

Mission:

- To understand the nature and Choice of methods of measurements.
- To learn the limits of detection and amplification.
- To demonstrate the concepts of Operational amplifiers.

Course outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO - 1	demonstrate automatic operation and computer control	1,5	Ap
CO - 2	precise control of current and voltage.	6,8	Ap
CO - 3	differentiate modulation and demodulation	5	An
CO - 4	point out limitation on amplifier performance	1	Cr
CO - 5	predict binary logic concepts, logic gates and multi-vibrators	7	Un
CO - 6	distinguish visual, filter and spectrophotometers.	6	Ap
CO - 7	control noise level in a system.	1,7	Cr
CO - 8	interpret the optimal value of adjustable parameters	7,8	Ev

Semester – I			
Elective I B Chemical Instrumentation			
Code : 19PCHE11	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Unit I Measurement and Instrumentation

Introduction - The nature of a measurement - Choice of a method of measurement - Control of variables - Basic design patterns - General properties of modules - Propagation of uncertainity - Single channel design - Limit of detection and amplification - Automatic operationand computer control.

Unit II Operational amplifiers

The operational amplifiers - Limitations on amplifier performance - Mathematical operations - Differentiation - Integration - Measurement of current and voltage - Precise control of current and voltage.

Unit III Signal-to-Noise Optimisation

Sensitivity and detection limits - Noise - Minimising Noise in a system - Signal averaging - Modulation: Chopping - Demodulation: Phase sensitive detection - Other methods ofOptimising Signal-to-Noise ratio.

Unit IV Digital Electronics

Binary logic concepts - Logic gates - Multivibrators - Counters - Wave shaping - Analog to digital convertors - Instruments and Digital computers.

Unit V Instrumentation for Optical Absorption Spectrometry

Visual Photometres - Filter Photometers - Spectrophotometer - Double beam Spectrophotometer - Recording Spectrophotometers - Optimal value of adjustable parameters - Multiple internal reflection assembly - Rapid scanning spectrometer - Non dispersive Photometers - Photometric titration equipment - Fourier transform Spectrometers.

Text book:

1. Strobel H A, Chemical instrumentation - A systematic approach to Instrumentational analysis, 2nd Edition, Addison- Wesley Publishing company Inc, Phillipines, 1973.

Books for reference:

1. Jeffery G H, Bassett J, Mendham J and Denney R C, Vogels Textbook of Qualitativechemical analysis, 5th Edition, Longman Scientific and technical, Essex, 1989.
2. Skoog D A, Hollar F J, Crouch S R, Principles of Instrumental analysis, 6th Edition, Thompson Brooks/ Cole, Belmont CA, 2007.

Semester – II			
Elective II A	**Energy and Environmental Chemistry**		
Code : 19PCHE21	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Vision:

To protect and improve the environment as a valuable asset against hazardous chemicals and energy resources.

Mission:

- To learn the various types of sonochemical reactions.
- To summarise renewable and non renewable energy resources.
- To gain knowledge about Environment and its problem solving techniques.

Course outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO - 1	compare heterogeneous liquid- liquid and heterogeneous solid- liquid reactions	2	An
CO - 2	distinguish between renewable and non- renewable energy resources.	5,6	An
CO - 3	explain the construction, working and applications of primary and secondary batteries.	4,8	Ap
CO - 4	classify and compare the fuels based on their appearance such as solid, liquid and gas.	7	Cr
CO - 5	demonstrate the Orsat process for flue gas analysis.	8	Ap
CO - 6	identify a catalyst used in fine chemical synthesis.	4,6	Un
CO - 7	sketch the natural cycles of environment such as the hydrological, oxygen and nitrogen cycles.	6	Cr
CO - 8	differentiate chemical and photochemical reactions occurs in atmosphere.	1,5	An

Semester – II			
Elective II A	**Energy and Environmental Chemistry**		
Code : 19PCHE21	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Unit I Sonochemistry

Introduction Instrumentation (Whistle reactor, Ultrasonic cleaning bath, Direct Immersion Sonic horn, The Cup horn) Types of Sonochemical reactions - Homogeneous reaction(Strecker, Solvolysis and Hydrolysis) - Heterogeneous liquid-liquid reactions (Hydrolysis, Solvolysis, Saponification and Esterification), Heteogeneous solid-liquid reactions, Induced Organic reactions (Bouveault reactions, Cannizzaro reaction, Strecker Synthesis, Reformatsky reaction, Barbier reaction of carbonyl compounds, Dickmann reaction)

Unit II Energy resources

Introduction - classification of energy resources - Renewable - Solar energy (Solar cells, Solar batteries, Solar heat collector and Solar water heater), Wind energy (Wind mills and Wind farms), Ocean energy (Tidal energy, Ocean thermal energy and geothermal energy) and Bio mass energy (Bio fuel and Hydrogen fuel).

Non Renewable - Batteries- Construction, Working and Applications: Primary battery - Leclanche Cell, Alkaline battery, Lithium ion; Secondary battery - NICAD, Lead Acid , Nickel metal hydride cell - Fuel cell - Use of alternate energy sources – Energy Conversion process: Anaerobic digestion and bio gas.

Unit III Fuels and combustion

Introduction - Classification of fuels - Calorific values - Solid fuel - Classification of coal by rank - Metallurgical coke and its manufacture (Otto Hoffmans method) - Liquid fuel - Petroleum - synthetic petrol and its manufacture (Bergius process) - Knocking - Octane number and Cetane number. Gaseous fuel - Liquid Petroleum gas, Natural gas, Compressed natural gas - Ignition temperature - Explosive range - Analysis of flue gas (Orsat process).

Unit IV Recent developments in catalysis

Introduction - Reactions over Solid - Acid catalyst (Alkylation, Cracking & Hydrocracking, Isomerisation), Catalyst in Fine Chemical synthesis (Halogenation, Amination, Condensation, selective Oxidation reactions), Photocatalyst - Introduction - Semiconductor as photocatalyst - Water splitting by Semiconductor Particle - Photocatalysis in the removal of Organic and Inorganic pollutants - Photocatalytic reduction of Dinitrogen, Photocatalysis of Organic reactions.

Unit V Environmental chemistry

Environmental Segments - The natural cycles of environment: the hydrological, oxygen and nitrogen cycles - Chemical and Photochemical reactions in atmosphere: SO_2, O_2 and O_3

chemistry, nitrogen oxides and organic compounds - Greenhouse effect - Ozone hole - El Nino phenomenon.

Microorganisms - the catalysts of aquatic chemical reactions - Acid-base and ion exchange reactions in soil - Nitrogen pathways and NPK in soil - Waste classification and disposal - Solid waste management.

Text Books:

1. Ahluwalia V.K & Varma R.S, Alternate Energy Process in Chemical Synthesis,1st Edition,Narosa Publishing House, Delhi, 2008.
2. Jain P.C and Monika Jain, Engineering Chemistry, 15th edition, Dhanpat Rai Publishingcompany Pvt. Ltd, New Delhi, 2011.

Books for Reference:

1. B.Viswanathan, S.Sivasanker, A.V.Ramaswamy, Catalysis-Principles and Applications,Fourth edition, Narosa Publishing House, Delhi, 2011.
2. Harish Kumar Chopra, Anupama Parmar, A textbook of Engineering Chemistry, NarosaPublishing House, 1st edition, New Delhi, 2008.
3. Dr.A.Ravikrishnan, Environmental Science & Engineering, Sri Krishna High tech Publishing Company Pvt. Ltd, Eleventh edition, 2015.
4. A.K.DE, Environmental Chemistry, New age international publishers, 6th edition, 2006.

Semester – II			
Elective II B	**Industrial Chemistry**		
Code : 19PCHE21	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Vision:

To develop better predictability of human health maintenance and prevention of various hazards.

Mission:

- To gain knowledge on industrial products.
- To create awareness regarding adulterants, radiation and its toxicity.

Course Outcome:

CO No.	Upon completion of this course, students will be able to	PSO addressed	CL
CO - 1	learn some of the industrial products like cosmetics, paints, dyes and pigments and their manufacturing	1, 5	An
CO - 2	test the adulterants present in cosmetics and take care of skin and hair	6	An
CO - 3	get to know various types of alloys and its manufacture and applications	5	Ap
CO - 4	have sufficient knowledge on corrosion and the methods for preventing corrosion	1, 5	Ap
CO - 5	discuss the basic concepts of radiation chemistry	1	An
CO - 6	understand the concepts, importance and need of nuclear energy	1	Ev
CO - 7	aware of disposal techniques of nuclear wastes and safety in working with nuclear energy	6	An
CO - 8	know various power projects in India.	7	An

Semester – II			
Elective II B	**Industrial Chemistry**		
Code : 19PCHE21	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

Unit I Cosmetics and Personal Care

Cosmetic formulations – Skin care - Hair care - Deodarants and Antiperspirants - Colour cosmetics - Sun protection aerosols - Nail cosmetics - Mouth cosmetics - Perfumes and fragrances.

Basic ingredients - Additives and flavours used in soaps, tooth pastes, lipsticks, perfumes, colognes, deodorants and antiperspirants - Harmful beautifying practices and their chemistry (Keratin depletion in hair – colouring - cleaning and curling of hair) - Basic tests for identifying good and bad cosmetics – pH Test.

Unit II Alloys and Corrosion

Alloys – Introduction - General characteristics of Alloys – manufacture – purpose of alloying - the Iron-Carbon Alloys - Carbon steels - Types of alloys - Heat treatment of alloys (Hardening of steel and Annealing) – Steel - Alloy steel – Stainless steel – Cast iron – Brass – Bronze – Nichrome.

Corrosion – Definition - Rusting of iron - Chemical corrosion - electrochemical corrosion - Factors influencing corrosion - Atmospheric and soil corrosion - Corrosion control - Hot dipping (galvanizing and tanning), Electroplating and Anodizing.

Unit III Pigments, Dyes and Paints

Pigments – Classification - Manufacture and uses of White lead, Lithopone, Ultramarine blue, Chrome green.

Dyes – Classification, preparation and dyeing processes.

Paints – Composition, manufacture and testing of paints - Special paints – temperature indicating paints, fire retardant paints, water repellant paints.

Unit IV Radiation Chemistry

Interaction of radiation with matter - primary effect due to charged particle - Radiation tracks, spurs and delta rays - linear energy transfer (LET) - Bethe's equation for LET for charged particles due to collisions with electrons - Radiation dosimetry - Units of radiation energy (Rad, Gray, Rontgen, RBE Rem, Sivert) - Radiolysis of water.

Unit V Applications of Nuclear chemistry and Trace elements

Chararacterisation of fission reactions - Product distribution, Theories of fission - Fissile and fertile isotopes - Synthetic elements - Nuclear reprocessing - Radiation hazards and prevention - Applications of isotopes - Neutron activation analysis - Isotopic dilution analysis -

Uses of traces in structural and mechanistic studies, agriculture, medicine and industry - Radiocarbon dating - Hot atom energy - Atomic power projects in India.

* **Students may visit Industries / premier Institutions.**

Text books:

1. Jain & Jain, Engineering Chemistry, S.Chand Publications, New Delhi, 2007.
2. Sharma B.K, Industrial Chemistry, Goel Publishing House, 2000.
3. Siva kumar.R, Siva Kumar. N, Engineering Chemistry, The Mc Graw-Hill companies,New Delhi, 2009.

Books for Reference:

1. Kirpal Singh, Chemistry in Daily Life, Prentice Hall of India Pvt. Ltd., New Delhi, 2nd Edn., 2008.

2. Charkarabarthy.B.N, Industrial Chemistry, Oxford and IBH Prb.Co., 2005.

3. Gopalan.R,Venkappayya .D, Sulochana Nagarajan, Engineering Chemistry II, VikasPublications, New Delhi, 2011.

4. V. Srinivasa, S.D.Uma Mageswari, M.Meena, Engineering Chemistry, ScietechPublications, 2002.

5. Arnikar.H.J, Essentials of Nuclear Chemistry, Wiley Eastern Ltd., 1988.