Course Name: Master of Science
Discipline : Chemistry
(For those who joined in June 2022 and after)

Course Outcome:

CO1: To provide adequate knowledge of various chemical phenomena including the recent developments in Chemistry.
CO2: To instill the confidence in students to do independent research work.
CO3: To ensure an excellent knowledge of applications in Chemistry.
CO4: To enable the students to get employed in the emerging/advanced fields of chemistry.
CO5: To enable the students to learn fundamentals, problem solving skills and apply.

Programme Outcomes

1. To provide a broad foundation in chemistry that stresses scientific reasoning and analytical problem solving with a molecular perspective.
2. To provide students with the skills required to succeed in competitive exams, the chemical industry, or professional school.
3. To expose the students to a breadth of experimental lab techniques using modern instrumentation.
4. To get advanced knowledge in chemistry.
5. To expose the interdisciplinary research aspect in chemistry.

Eligibility for admission:

The candidates should have a Bachelor Degree in Chemistry from Madurai Kamaraj University or from any other University recognized by the syndicate of Madurai Kamaraj University.

Duration of the course: Two years

Medium of Instruction and Examination:

The medium of instruction as well as the examination will be English.

Course Scheme:

VIRUDHUNAGAR HINDU NADARS' SENTHIKUMARA NADAR COLLEGE
(An Autonomous Institution Affiliated to Madurai Kamaraj University)
[Re-accredited with 'A' Grade by NAAC]
Virudhunagar – 626 001.

Semester	Subject	Hr	Cr	Int+Ext = Total	Local	Regional	National	Global	Professional Ethics	Gender	Human Values	Environment & Sustainability	Employability	Entrepreneurship	Skill Development	Subject Code	Revised / New / No Change / Interchanged & Percentage of revision
I	Core Subject I – Organic Chemistry I	5	5	40+60=100				✔	✓				✓			**P22CHC11**	10 % revised
	Core Subject II – Inorganic Chemistry I	5	4	40+60=100				✔	✓				✓			**P22CHC12/** P19CHC12	No Change
	Core Subject III – Physical Chemistry I	5	4	40+60=100				✔	✓				✓			**P22CHC13**	30 % revised
	Core I – LAB: Organic Chemistry Practical I	3	-	-----				✔	✓						✓	-	Interchanged
	Core II – LAB: Inorganic Chemistry Practical I	4	-	-----				✔	✓						✓	-	No Change
	Core III – LAB: Physical Chemistry Practical I	4	-	------				✔	✓						✓	-	No Change
	Major Elective 1 – Nano science and Nanotechnology/ Computer in Chemistry	4	4	40+60=100				✔	✓				✓			**P22CHE11/ P22CHE12**	75 % revised
II	Core Subject IV – Organic Chemistry II	5	4	40+60=100				✔	✓				✓			**P22CHC21**	10 % revised
	Core Subject V – Inorganic Chemistry II	5	5	40+60=100				✔	✓				✓			**P22CHC22/** P19CHC22	No Change
	Core Subject VI – Physical Chemistry II	5	4	40+60=100				✔	✓				✓			**P22CHC23**	30 % revised
	Core I – LAB: Organic Chemistry Practical I	3	3	40+60=100				✔	✓						✓	**P22CHP21/** P19CHP21	No Change
	Core II – LAB: Inorganic Chemistry Practical I	4	4	40+60=100				✔	✓						✓	**P22CHP22/** P19CHP22	No Change
	Core III – LAB: Physical Chemistry Practical I	4	4	40+60=100				✔	✓						✓	**P22CHP23/** P19CHP23	No Change
	Non-Major Elective – Industrial Chemistry / Applied Chemistry	4	4	40+60=100				✔	✓				✓			**P22CHN21/ P22CHN22**	20% revised

SEMESTER-I

PART–III- CORE SUBJECT I- ORGANIC CHEMISTRY I

Hours per week: 5 **Credits: 5** **Subject Code: P22CHC11**

Course Outcomes

On completion of course the student can knew

CO 1: To study the mechanism of organic reaction.

CO 2: To Study the reaction intermediates and theory behind it.

CO 3: To provide the knowledge about the stereochemistry and geometry of the molecule.

CO 4: To give basics knowledge on the aromatic character of organic molecules.

CO 5: To acquire the knowledge about the detail study of UV, IR and Mass spectroscopy.

UNIT I: Electron displacement and structure – reactivity correlation **15 Hours**

Inductive and field effects– bond distances – bond energies – delocalized bonds – cross conjugation– rules of resonance – resonance energy – resonance effect – steric inhibition of resonance – Hyper conjugation – hydrogen bonding – effect of structure on the dissociation constants of acids and bases – HASB concepts. Quantitative treatment of the effect of structure on reactivity– The Hammett relationship – significance of reaction and substituent constants – application of the Hammett equation in reaction mechanism – limitations and deviations- Taft equation.

Unit II: Introduction to reaction mechanism **15 Hours**

Reaction intermediates – free radicals, carbenes, nitrenes, carbanions, carbocations – formation and stability of reaction intermediates– methods of determination of reaction mechanism – kinetic and thermodynamic control of chemical reactions - Intermediate versus transition state-Analysis of product and intermediate-Isotopic labelling –Stereo chemical studies-Cross over experiment-Kinetic methods-Isotopic and substituent effects. Kinetic and non-kinetic methods for determining organic reaction mechanism– principle of microscopic reversibility – energy profile diagram – Hammond postulate.

Unit III: Stereochemistry **15 Hours**

Concept of chirality, necessary and sufficient conditions for chirality – relationship between substrate symmetry and chirality. Projection formulae – Wedge, Fischer, Sawhorse and Newmann. Optical isomerism due to centre of chirality. Molecules with one stereogenic centre (chiral centre) and molecules with more than one chiral centre. Erythro and threo nomenclature. Configuration – determination of configuration. Cahn, Ingold and Prelog system (R-S) of designation of configuration (aliphatic, cyclic and polycyclic molecule).

Prochirality and prostereoisomerism, enantiotopic and diasterotopic ligands and faces and their nomenclature– pro-R and pro-S and Re and Si faces, stereospecific and stereoselective reactions. Asymmetric synthesis; Cram and Prelog rules. Optical isomerism due to axial chirality – biphenyls, allenes and spiranes. Molecules with planar chirality – paracyclophanes, *trans* cyclooctene, ansa compounds.

E-Z nomenclature– determination of configuration of geometrical isomers using physical and chemical methods– stereoisomerism in monocyclic compounds (upto six membered ring).

Unit IV: Aromatic character **15 Hours**

Aromatic character in benzene, six membered rings, five, seven and eight membered rings – other systems with aromatic sextets – Huckel's rule – Craig's rule – concept of

homoaromaticity and antiaromaticity – systems with 2,4,8 and 10 electrons – systems with more than 10 π electron – Mobius aromaticity- Alternant and nonalternant hydrocarbons. Chemistry of cyclo pentadienyl anion – Fulvene, Azulene, Tropolones, Sydnones and Annulenes.

Novel ring systems

Nomenclature of bicyclic and tricyclic systems – chemistry of adamantane, diamantane (congressane), cubane and catenanes.

Unit V: Spectroscopy I

UV Spectroscopy: 15 Hours

Principle – Factors influencing UV-absorption spectra - absorption spectra of conjugated dienes – α, β unsaturated Carbonyl compounds – Woodward – Fieser rules- Applications of UV-spectra.

IR Spectroscopy: Molecular vibrations – vibrational frequency – factors influencing group frequencies – quantitative studies- Applications of IR spectra.

Mass Spectroscopy: Principle– type of ions – base peak – parent ion , metastable and isotopic peaks – fragmentation – general rules – pattern of fragmentation for various classes of compounds – McLafferty rearrangement – Retro Diels – Alder reaction.

Text/Reference Books

Unit – I , II, III & IV

1. P.Sykes, Guidebook to Mechanism in Organic Chemistry, Orient Longmann Ltd., New Delhi, 1998.
2. Jerry March, Advanced Organic Chemistry, John Wiley and Sons, 4th edition, 2004.
3. E.S. Gould, Mechanism and Structure of Organic Chemistry, Holt, Rinehart and Winston Inc, New York, 1959.
4. J. Shorter, Correlation Analysis in Organic Chemistry, Clarendon Press, Oxford, 1973.
5. R.T. Morrison and R.N. Boyd, Organic Chemistry, Prentice – Hall, 6th edition, 2001.
6. I.L Finar, Organic Chemistry Vol. I and II , 6th edition, John Wiley and Sons, New York, 2000.
7. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, Harper Collins, 1987.
8. Reinhard Bruckner, Advanced Organic Chemistry, Reaction Mechanisms, Academic Press, 2002.
9. F.A Carey and R.J. Sundberg , Advanced Organic Chemistry, Part B, 5th edition, Springer Publishers, 2008.
10. R. E. Ireland, Organic synthesis, Prentice - Hall of India Pvt. Ltd., 1975.

Unit- V

1.William Kemp, Organic Spectroscopy , ELBS , 3rd edition, 2011.
2.John R.Dyer, Application of Absorption Spectroscopy of Organic Compounds, 3rd edition, ELBS, 1987.
3.Robert M.Silverstein and Francis X.Webster, Spectrometric Identification of Organic compounds, 6th edition, Wiley and Sons, Inc, 2010.
4.P.S.Kalsi, Spectroscopy of Organic Compounds, 6th edition, New Age International Publishers, 2009.
5.Jag Mohan, Organic Analytical Chemistry – Theory and Practice, Narosa Publishing House,2003.
6.Jag Mohan, Organic Spectroscopy, Principles and Applications, 2nd edition, Narosa Publishing House, 2010.

e-Resources

1. https://en.wikipedia.org/wiki/Adamantane#.
2. https://en.wikipedia.org/wiki/Diamantane
3. https://en.wikipedia.org/wiki/Cubane
4. https://en.wikipedia.org/wiki/Catenane
5. http://dl.iranchembook.ir/ebook/organic-chemistry-2747.pdf
6. https://www.khanacademy.org/science/organic-chemistry/spectroscopy-jay

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PART–III- CORE SUBJECT II- INORGANIC CHEMISTRY I

Hours per week: 5 **Credits: 4** **Subject Code: P22CHC12/** P19CHC12

Course Outcome:

CO1 : Be able to predict molecular geometries and bond properties with the help of bonding theories.
CO2 : Analyse the effect of non-bonding electrons in molecular structures.
CO3 : Be able to learn about formation, structure and bonding of inorganic polymers.
CO4 : Acquire knowledge about the basics of co-ordination chemistry.
CO5 : Be able to know about the metallurgical process.

Unit I: Bonding theory **15 Hours**

Qualitative treatment of VB and MO theories– σ and π bonds – hybridization and resonance – MO equivalent of hybridization – application of VB and MO theories to the structures of homonuclear and heteronuclear diatomic (CO, HF and HCl) and triatomic molecules ($BeCl_2$ and H_2O) – comparison of VB and MO theories. VSEPR theory – bonding in xenon compounds.

Unit II: Bond properties and ionic bonding **15 Hours**

Ionic radius –covalent radius – van der Waals radius. Bond order, bond energy, bond length–bond polarity – partial ionic character – electronegativity – electron affinity – lattice energy –Born Lande equation, Kapustinskii equation. Born Haber cycle – covalent character in ionic compounds – different types of electrostatic interactions – hydrogen bonding.

Unit III: Inorganic chains, rings and cages **15 Hours**

Polyacids – classification – isopoly acids like polymolybdate, polyvanadate and polytungstate– their structures – heteropolyacids 12A, 12B, 9 and 6 heteropolyacids – preparation and structure of Borazine. Phosphazenes and their polymers – phosphonitrilic compounds – S_4N_4 – polymeric sulphur nitride (polythiazyl) cage compound. Boranes – nomenclature of boranes and carboranes –Wade's rules – Styx number – preparation and structures of B_2H_6, B_4H_{10} and $C_2B_{10}H_{12}$.

Unit IV: Coordination chemistry I **15 Hours**

IUPAC nomenclature of coordination compounds – isomerism in coordination compounds – types of ligands – monodentate, ambidentate and macrocyclic ligands – chelate and its applications – detection of complex formation in solution – stability constant – thermodynamic stability and kinetic stability – stepwise stability constant and overall stability constant and the relationship between them - factors affecting stability constant in solution – determination of stability constant by spectrophotometric (Job's methods), polarographic and potentiometric methods.

Unit V: Metallurgy **15 Hours**

Occurrence, extraction, purification, properties and uses of the following metals as well as their important compounds: Ti, Zr, V, U, Be, Th and Ge. Platinum group metals

(general extraction only). Different forms of Pt – Preparation and uses.

Text/Reference books

Unit I - IV

1. J.E.Huheey, E.A.Keiter, R.L.Keiter and O.K.Medhi**,** Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, Pearson Education Inc., 2006.
2. F.A.Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 6th edition, John Wiley and Sons, New York, 2009.
3. J.D. Lee, Concise Inorganic Chemistry, 5th edition, Blackwell Science Ltd., Oxford, 2000.
4. D.F.Shriver and P.W.Atkins, Inorganic Chemistry, 4th edition, Oxford Univ. Press, 2009.
5. R.Gopalan and V. Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd., New Delhi 2010.
6. Satya Prakash, G.D.Tuli, S.K.Basu and R.D.Madan, Advanced Inorganic Chemistry Volume – I & II, S.Chand and Company PVT Ltd, 2008.

Unit V

1. H.D. Mathur and O.P.Tandon, Chemistry of Rare Elements, 3rd edition, S.Chand and Co., 1989.
2. Satya Prakash, Advanced Chemistry of rare elements, S.Chand and Company PVT Ltd, 2013.

e – Resources

1. https://byjus.com/jee/molecular-orbital-theory/
2. https://www.youtube.com/watch?v=nTujP4jCbsg
3. https://testbook.com/learn/chemistry-vsepr-theory/
4. https://byjus.com/jee/chemical-bonding/
5. https://www.dalalinstitute.com/wp-content/uploads/Books/A-Textbook-of-Inorganic-Chemistry-Volume-1/ATOICV1-5-0-Isopoly-and-Heteropoly-Acids-and-Salts.pdf

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PART III – CORE SUBJECT III – PHYSICAL CHEMISTRY I

Hours per week: 5 **Credits: 4** **Subject Code: P22CHC13**

Course Outcome

CO1: Will be in a position to explain the theoretical concepts of quantum mechanics, thermodynamics, chemical equilibria and phase equilibria.

CO2: Will be able to apply the knowledge of quantum mechanics to solve simple quantum mechanical problems and to illustrate the applications of thermodynamic parameters.

CO3: Will be able to interpret the advanced knowledge on quantum concepts to evaluate the shapes of orbitals as well as to identify the various energy levels in molecular systems andto utilize the thermodynamical functions to understand Lechatelier's principle and phasetransition studies.

CO4: Can calculate various molecular energy levels using principles of quantum mechanics and derive thermodynamic relations.

CO5: Can establish the applications of various mathematical operations in quantum mechanics and to assess the relation between the thermodynamic parameters and variety of reactions.

Unit I: Quantum mechanics –An introduction **15 Hours**

Basic principles of quantum mechanics:Planck's quantum theory, wave particle duality, uncertainty principle; Postulates of quantum mechanics – Operator algebra: Expressions – addition, subtraction and multiplication– linear operators – Laplacian operator – vector operator – ladder operator – quantum mechanical operator for the following observables: position, momentum, kinetic energy, potential energy, total energy and angular momentum – commutator algebra – evaluation of commutators – commutation rule for angular momentum – Hermitian operator – properties of Hermitian operator – properties of wave functions – Eigen function – Eigen value – Concept of orthogonality and normalization significance of ψ and ψ^2.

Unit II: Application of quantum mechanics to simple systems **15 Hours**

Derivation of Schrodinger wave equation – Setting up and solving Schrodinger wave equation and arriving solution for particle in one dimensional box, Particle in a ring, 3D cubical box, 3D rectangular box, the harmonic oscillator, the rigid rotator and the hydrogen atom; Degeneracy and degenerate wave functions; Quantum mechanical tunneling- Radial probability distribution curves and shapes of atomic orbitals

UNIT III: Thermodynamics – I **15 Hours**

Brief resume of concepts of First law and Second law of Thermodynamics; Thermodynamic equations of state in terms of internal energy & in terms of enthalpy- application of these equations to ideal and non-ideal gases; Gibbs free energy function – Prediction of direction and occurance of a process in terms of ΔH, ΔS and ΔG; Temperature dependence of ΔG & ΔA- Gibb's Helmholtz equation in its integrated form and its applications & limitations; Standard reaction free energy – its determination from thermochemical, electrochemical and equilibrium data; Clapeyron equation - Clausius – Clapeyron equation and its applications; Maxwell's thermodynamic relations.

UNIT IV: Thermodynamics – II **15 Hours**

Concepts of partial molar properties – 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; Third law of Thermodynamics – Absolute entropies – Determination of Absolute entropies – Exception to Third law - Unattainability of absolute zero – Zeroeth law of thermodynamics.

UNIT V: Chemical and phase equilibria **15 Hours**

van't Hoff reaction isotherm for equilibrium involving ideal and non-ideal gases – K_P, K_C & K_X and relationship among them - Temperature coefficient of reaction free energy and equilibrium constant – van't Hoff reaction equation – Problems – De-Donder's treatment of chemical equilibria – Thermodynamic explanation of Lechatelier's principle – The Hammet equation as a linear free energy relationship.

Gibbs Phase rule and Lever rule-Derivation of phase rule from the concept of chemical potential. Application of phase rule to three component systems - Plots for a mixture of three liquids consisting of one, two and three pairs of partially miscible liquids.

TEXT BOOKS

1. A. K. Chandra, Introductory Quantum Chemistry, 3rdEdition, Tata-McGraw Hill Pub. Co., New Delhi, 1988.
2. D.N. Bajpai, *Advanced Physical Chemistry*, New Delhi**:** S.Chand& Co.,Ltd.,1st Edition (2011).
3. B.R. Puri**,** L.R. Sharma and M.S. Pathania (2003) *Principles of Physical Chemistry.*New Delhi **:**Vishal Publishing Co**,** 1st Edition.

4. J.N. Gurtu and A. Gurtu, Advanced Physical Chemistry, Pragati Prakashan Pub., Eighteenth Edn., (2015).
5. S. H. Maron, J. B. Lando& C.F Prutton, Fundamentals of Physical Chemistry, Macmillon, New York (1974)

.**Reference Books**

1. D. A. McQuarrie, Quantum Chemistry, 1st Indian Edition, Viva Books (P) Ltd., New Delhi, 2003.
2. H.W. Hanna, Quantum Mechanics in Chemistry, Benjamin / Cummings Pub. Co., London, 1983.
3. I.N. Levine, Quantum Chemistry, 4th edition, Prentice-Hall India, New Delhi, 2000.
4. R.K. Prasad, (2000). *Quantum Chemistry*,New Delhi: New Age International publishers, 4th Edition.
5. E. House, *Fundamentals of Quantum Chemistry*,California: Academic Press, 2nd Edition (2008).
6. S.Glasstone, Thermodynamics for Chemists, East-West Press Private Ltd., New Delhi, 1969.
7. J. Rajaram and J. C. Kuriakose, Thermodynamics, 3rd edition, S. Chand & Co. Ltd., 1986.
8. D. A. McQuarrie and J.D. Simon, Physical Chemistry - A Molecular Approach, Viva Books (P) Ltd., New Delhi, 1998.
9. GurdeepRaj,S.(2003). *Advanced Physical Chemistry*. Meerut: Goel Publishing Co.25th Edition.
10. P.W. Atkins, and J.D. Paula, (2012). *Physical Chemistry*. New York: ELPS and Oxford University press, 7th Edition.

e- Resources

1. https://youtube.com/channel/UCb1gintRG37w6-CAaGRm4Mg
2. https://youtube.com/playlist?list=PLOzRYVm0a65eW1kTGOrjBetXFMl4eaYVi - Quantum Mechanics
3. http://www.freebookcentre.net/Physics/Quantum-Mechanics-Books.html - Quantum Mechanics Book link
4. https://nptel.ac.in/courses/103/101/103101004/#watch Thermodynamics
5. https://nptel.ac.in/content/storage2/courses/112105129/pdf/RAC%20Lecture%204.pdf Thermodynamics

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MAJOR ELECTIVE I - NANO SCIENCE AND NANOTECHNOLOGY

Hours per week: 4 **Credits: 4** **Subject Code: P22CHE11**

Course Outcomes:

CO1: Understood the principles and background to nanotechnology.
CO2: Understand the basics properties of nanomaterial.
CO3: Make the students to acquire knowledge for the synthesis of nanomaterials.
CO4: Understood the principles and characterization techniques of nanomaterials.
CO5: Ability to identify tailor made nano applications for developing nanotechnology.

Unit I: Classification and properties of Nanomaterials **12 Hours**

Definition of Nanomaterials and nanotechnology - Classification of nanostructure materials: 0D, 1D - nanowires, 2D – nanorods, nanotubes, 3D and nanofluids - Surface effects of Nanomaterials - Carbon nanostructure: Fullerenes, carbon nanotubes-Metal oxides nanoparticles: Zinc oxide, Aluminium oxide, Nickel oxide, Cobalt oxide and Copper oxide. Properties of nanomaterials: Optical properties, Surface plasmon resonance effect, quantum

size effects - Electrical properties, dielectric materials – Magnetic properties, superparamagnetism - electrochemical properties and chemical sensing properties.

UNIT-II: Methods of Generation of Nanomaterials 12 Hours

General approaches synthesis of nanomaterials: Bottom up and top down approaches – Techniques for the synthesis of nanomaterials - Physical techniques: Laser ablation, Aerosol synthesis, Ball milling technique, Chemical vapour deposition and Plasma synthesis method – Chemical approaches: Solvothermal synthesis, hydrothermal synthesis, Micro-emulsion method, Sol-gel synthesis and Sonochemical process.

Unit III: Electron Microscopy Techniques for Surface image Analysis . 12 Hours

Principles of Electron Microscopy- difference between optical microscope and electron microscope- Scanning Electron Microscope: instrumentation, imaging and crystallographic information, strength and limitation of SEM – Energy dispersive X-ray analysis (EDX)- Transmission Electron microscope: instrumentation: TEM specimen preparation, Quantitative analysis using TEM – Atomic force microscopy: Principles, instrumentation, contact mode, non-contact mode and tapping mode, comparison of AFM and other imaging techniques – Principles and instrumentation of X-ray photoelectron spectroscopy (XPS).

Unit IV: X-ray Diffraction and Spectroscopic techniques. 12 Hours

Principle and instrumentation of XRD, The powder method, determination of grain size and crystallite size, XRD pattern analysis of some commercially metal oxides -Infra red spectroscopy - UV-Visible spectroscopy:Tauc's plot, characterization of materials and Nanoparticles- Raman spectroscopy: carbon based Nanomaterials, nanomaterials from metals -Photoluminescence: operating principle, instrumentation, spectrum and interpretation– Cathodoluminescence.

Unit V: Application of nanomaterials 12 Hours

Application of nanomaterials: Nanomaterials in medicine: diagnosis and therapeutic agent – Applications of nanomaterials in energy sector: Hydrogen production and conversion (photoelectrochemical cells and fuel cells), Nanomaterial in energy storage (Batteries and supercapacitors)-Water treatment and the environment application : heavy metal removal and photocatalytic decontamination- Nanocatalysts: acid catalysis, base catalysis and biocatalysis – Food, textile industry and agricultural industry

Text Books:

Unit I

1. B.Viswanathan, Nano Materials, published by Narosa publishing house Pvt.Ltd, New Delhi (2011), (Page No: 1.1-1.2, 2.5-2.10,).
2. M.A. Shah and T. Ahmad , Principles of Nanoscience and Nanotechnology, published by Narosa Publishing House, NewDelhi, (2010), (page No: 5-10, 15-28, 138-152).
3. B.S. Murty, P. Shankar, Baldev Raj, B.B. Rath and Murday.Textbook of Nanoscience and Nanotechnology, published by University Press (India) private limited, Hyderabad, (2012), (Page No: 3-8, 10-16, 29-65).

Unit II

1. M.A. Shah and T. Ahmad , Principles of Nanoscience and Nanotechnology, published by Narosa Publishing House, NewDelhi, (2010), (page No: 32-65).
2. B.S. Murty, P. Shankar, Baldev Raj, B.B. Rath and Murday.Textbook of Nanoscience and Nanotechnology, published by University Press (India) private limited, Hyderabad (2012), (Page No: 66-85).

Unit III

1. M.A. Shah and T. Ahmad , Principles of Nanoscience and Nanotechnology, published by Narosa Publishing House, NewDelhi, (2010), (page No: 67-91).

2. B.S. Murty, P. Shankar, Baldev Raj, B.B. Rath and Murday.Textbook of Nanoscience and Nanotechnology, published by University Press (India) private limited, Hyderabad (2012), (Page No: 152-170).

Unit IV

1. M.A. Shah and T. Ahmad , Principles of Nanoscience and Nanotechnology, published by Narosa Publishing House, NewDelhi, (2010), (page No: 111-125)
2. B.S. Murty, P. Shankar, Baldev Raj, B.B. Rath and Murday.Textbook of Nanoscience and Nanotechnology, published by University Press (India) private limited, Hyderabad (2012), (Page No:149 & 150).
3. https://www.jove.com/t/61764/uv-vis-spectroscopic-characterization-nanomaterials-aqueous (PriscilaAlessio, Pedro H.B. Aoki, Leonardo N. Furini, Alvaro E. Aliaga, Carlos J. Leopoldo Constantino) page No: 65-85.

Unit V

1. B.Viswanathan, Nano Materials, published by Narosa publishing house Pvt.Ltd, New Delhi (2011), (Page No: 2.1-13.32).
2. M.A. Shah and T. Ahmad , Principles of Nanoscience and Nanotechnology, published by Narosa Publishing House, NewDelhi, (2010), (page No: 158-185).
3. B.S. Murty, P. Shankar, Baldev Raj, B.B. Rath and Murday.Textbook of Nanoscience and Nanotechnology, published by University Press (India) private limited, Hyderabad (2012), (Page No: 167-210).

References books:

1. Nanostructures and Nanomaterials - Synthesis, Properties and Applications - Cao, Guozhong Imperial College Press (2004) London.
2. Rao, C.N.R., Müller, A. and Cheentham, A.K. (Eds.),"Chemistry of Nanomaterials", Wiley – VCH. 2005
3. Schmid, G. (Ed.), "Nanoparticles", Wiley-VCH Verlag GmbH & Co. KgaA 2004.
4. Klabunde, K.J. (Ed.), "Nanoscale Materials in Chemistry", John Wiley & Sons Inc. 2001
5. T. Pradeep, Understanding Nanoscience and Nanotechnology, Tata McGraw-Hill Education (2007), New Delhi.

e- Resources

1. http://nupex.eu/index.php?g=textcontent/materialuniverse/sizeofthings&lang=en
2. http://www.slideshare.net/niraliakabari3/ppt-of-phynanophysics
3. http://www.nanoscienceworks.org/publications/books/4/9781420048056/instruct
4. ors/ITNS-Lecture-1.pdf
5. http://ipn2.epfl.ch/lns/lectures/nanoscience/lecturenotes/cour-1.pdf 5.
6. www.uniroma2.it/didattica/NANOSCIENZE/deposito/L1.ppt
7. mp.misis.ru/docs/courses/17/Mats_Moscow_2.ppt 6.
8. http://uw.physics.wisc.edu/~himpsel/Nano/lectures.htm
9. www.nptel.ac.in
10. www.mit.co.in

SEMESTER II

PART III– CORE SUBJECT IV –ORGANIC CHEMISTRY II

Hours per week : 5 **Credits:4** **Subject Code: P22CHC21**

Course Outcomes:

On completion of course the student can knew

CO 1: To study the relationship between conformation and reactivity of organic molecules.

CO 2: To study the NMR Principles, spectral problems solving and interpretation of organic molecules .

CO 3: To acquire the knowledge about the addition reactions and organic naming reactions

CO 4: To get knowledge about the aliphatic substitution reactions of organic compounds.

CO 5: To develop the aromatic substitutions and elimation reactions of organic compounds.

Unit I: Conformational analysis **15 Hours**

Configuration and conformation– conformations of ethane, n-butane and 1,2 – dichloroethane– conformation analysis – stereo electronic and steric factors – conformation of simple acyclic compounds – conformation of cyclohexane and its monosubstituted and disubstituted derivatives, conformation of decalin system – correlation of the conformation of acyclic and cyclic systems with their physical and chemical properties– conformational free energy – Curtin-Hammett principle – quantitative treatment of mobile system – Eliel-Ro equation – conformations and reactivity of cyclohexanones – conformational analysis of aldohexopyranoses.

Unit II: NMR Spectroscopy **15 Hours**

^{1}H NMR Spectroscopy

Origin of NMR spectra – chemical shift – spin-spin coupling – coupling constant – first and second order spectra– influence of stereochemical factors on chemical shift of protons – simplification of complex spectra – deuterium substitution – spin decoupling – double resonance – shift reagents – Nuclear Overhauser Effect – CIDNP NMR.

^{13}C NMR Spectroscopy

Basic principle of FT technique– Relaxation time – assignment of signals – Off Resonance Decoupling – additivity relationship – calculation of chemical shifts for aromatic and aliphatic compounds – DEPT, COSY and HETCOR. Composite problems involving UV-Vis, IR, NMR and Mass spectra.

Unit III: Addition to multiple bonds **15 Hours**

Electrophilic, nucleophilic and free radical additions – Electrophilic addition- one step mechanism - two step mechanism- termolecular addition - addition to conjugated systems – orientation of the addendum - Markovnikov addition and peroxide effect (Free radical addition) – stereochemical factors in reactions like addition of hydrogen (syn and anti addition), halogens (Stereo specific and Stereo selective reaction), hydrogen halides and hypohalous acids, hydroboration (Regiospecific reaction) – hydroxylation by OsO_4 and Bayer's reagent (syn addition) – epoxidation (anti addition). Nucleophilic addition- difference between electrophilic and nucleophilic addition - Addition to carbonyl groups – mechanism – Aldol condensation – Perkin reaction – Knoevenagel reaction –Mannich reaction – Cannizaro reaction – Benzoin condensation– Claisen ester condensation – Darzen's reaction – Reformatsky reaction – Wittig reaction– Grignard reactions-abnormal

Grignard addition. Addition to α,β-unsaturated carbonyl compounds – Michael addition – Diels-Alder reaction – Esterification of acids and hydrolysis of esters– decarboxylation of carboxylic acids.

Unit IV: Aliphatic substitution reactions **15 Hours**

Aliphatic nucleophilic substitution

Nucleophilicity and basicity – S_N1 and S_N2 mechanisms – effect of substrate structure – effect of attacking nucleophiles, leaving groups and reaction medium – ambident nucleophiles – ambident substrates - Comparison of S_N1 , S_N2 and S_Ni – neighbouring group participation of n, π and σ electrons – S_Ni mechanism – nucleophilic substitution at an aliphatic trigonal carbon – nucleophilic substitution at an allylic carbon – nucleophilic substitution at a vinyl carbon.

Aliphatic electrophilic substitution

Electrophilic substitution at saturated carbon– S_E1 , S_E2 and S_Ei mechanisms.

Unit V: Aromatic substitution and Elimination reactions **15 Hours**

Aromatic electrophilic substitution – orientation and reactivity – mechanism of nitration, halogenation, Friedel-Craft's reaction and sulphonation – partial rate factors –ortho / para ratio – Quantitative treatment of reactivity of electrophiles (the selectivity relationship) – Aromatic nucleophilic substitution reactions – S_NAr, S_N1 and benzyne mechanisms.

Elimination reactions: α-Elimination, β-elimination, E1, E2 and E1cB mechanism– stereochemistry of elimination – orientation of the double bond (Saytzeff's rule and Hofmann elimination) – effect of changes in the substrate, base, leaving group and medium on E1, E2, E1cB reactions – elimination *vs* substitution – pyrolytic *cis* elimination – Bredt's rule.

Reference books

Unit – I, III, IV & V

1. I.L. Finar, Organic Chemistry, Vol. II, 6th edition, John Wiley and Sons, New York,2000.
2. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, Harper Collins, 1987.
3. Jerry March, Advanced Organic Chemistry, John Wiley and Sons, 4th edition, 2004.
4. E.S. Gould, Mechanism and Structure of Organic Chemistry, Henry, Rinehart and Winston, New York, 1959.
5. Reinhard Bruckner, Advanced Organic Chemistry, Reaction Mechanisms, Academicpress, 2002.
6. F.A.Carey and R.J. Sundberg, Advanced Organic Chemistry, Part B, 5th edition, plenum Publishers, 2008.
7. P. Ramesh, Basic Principles of Organic Stereochemistry, I Ediion, Meenu Publications, 2005.
8. P.S. Kalsi, Stereochemistry: Conformation and mechanism, 10th edition, New Age International Publishers, 2019.
9. E. L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw - Hill Edition, 2004.
10. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 4th Edition, New Age International Publishers, 2021.

Unit -II

1. John R.Dyer, Application of Absorption Spectroscopy of Organic Compounds, 3rd edition, ELBS, 1987.
2. William Kemp, Organic Spectroscopy , ELBS , 3rd edition, 2011.
3. Robert M.Silverstein, Francis X. Webster, Spectrometric Identification of Organic

compounds, 6th edition, John Wiley and Sons Inc., 2010.
4. P.S.Kalsi, Spectroscopy of Organic Compounds, 6th edition, New Age International Publishers, 2009.
5. Jag Mohan, Organic Analytical Chemistry – Theory and Practice, Narosa Publishing House, 2003.
6. Jag Mohan, Organic Spectroscopy, Principles and Applications, 2nd edition, Narosa Publishing House, 2010.

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1. https://byjus.com/chemistry/nmr-spectroscopy/
2. https://www.jeol.co.jp/en/products/nmr/basics.html
3. https://new.bhu.ac.in/Content/Syllabus/Syllabus_30063128202004140356 42.pdf
4. https://www.alfa.com/en/named-reactions-in-organic-synthesis
5. https://www.siue.edu/~tpatric/NS.pdf
6. https://byjus.com/jee/nucleophilic-substitution-reaction/
7. https://www.chemistrysteps.com/nucleophilic-aromatic-substitution/

PART III – CORE SUBJECT V – INORGANIC CHEMISTRY II

Hours per week: 5 **Credits: 5** **Subject Code: P22CHC22/** P19CHC22

Course Outcome:

CO1: Be able to predict molecular geometries of the coordination compounds with the help of bonding theories
CO2: Understand the formation structure and bond properties of metal carbonyls
CO3: Be able to learn the applications of metal carbonyls in industrial process
CO4: Acquire knowledge about the reaction mechanism of co-ordination compounds
CO5: Be able to know about the effect of rearrangement in inorganic complexes

Unit I: Coordination Chemistry II 15 Hours

Theory of bonding – VB, CFT and MO theories – splitting of d-orbitals in Oh, Td, square planar, trigonal bipyramidal and square pyramidal geometries– tetragonal distortion – Jahn-Teller Effect – CFSE calculation in terms of Dq – factors affecting crystal field splitting – spectrochemical series – application of CFSE – MO diagram of octahedral complexes – effect of π-donor and π-acceptor ligands – magnetic properties of transition metal complexes– calculation of spin only magnetic moments – orbital contribution to the magnetic moment – spin orbit coupling.

Unit II: Complexes of π-acceptor ligands 15 Hours

Introduction – EAN rule and its correlation to stability. Synthesis, structure and bonding in metal carbonyls, nitrosyls and dinitrogen complexes – IR study of metal carbonyls and nitrosyls. Synthesis, properties, structure and bonding in ferrocene, olefin and allyl complexes.

Unit III: Reaction mechanism of coordination compounds 15 Hours

Substitution reactions of octahedral complexes – labile, inert complexes – mechanism of acid hydrolysis – base hydrolysis and anation reaction – substitution reactions of square planar complexes – factors affecting reactivity of square planar complexes – trans-effect – π bonding and polarization theories – applications of trans effect – electron transfer reactions – complementary and non complementary reactions – outer sphere and inner sphere electron transfer mechanisms.

Unit IV: Organometallic catalysis 15 Hours

Homogeneous catalysis involving organometallics– oxidative addition – reductive

elimination – insertion reaction – Wilkinson catalyst, Waker process and hydroformylation carbonylation of alcohols. Heterogeneous catalysis – Ziegler-Natta polymerization. Cyclooligomerisation of acetylenes (Reppe's and Wilkei's catalysis) – Fischer Tropsch synthesis. Water gas shift reaction – Synthetic gasoline (Fischer Tropsch and Mobile process)

Unit V: Molecular rearrangement reaction of coordination complexes 15 Hours

Molecular rearrangement of four coordinated complexes - six coordinated complexes - reactions at coordinated ligands – reaction due to metal ion polarization of coordinated ligands - hydrolysis of amino acid esters, amides and peptides – aldol condensation – imine formation - the template effect and macrocyclic ligands.

Reference books

Unit – I

1. B.N.Figgis, Introduction to Ligand Fields, Interscience Publishers, New York, 1967.
2. S.F.A. Kettle, Coordination Compounds, ELBS, 1975.
3. R.Gopalan and V. Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd., New Delhi 2010

Unit - II

1. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, W.B. Saunders Company, 1977.
2. R.Gopalan and V. Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd., New Delhi 2010

Unit – III

1. R.Gopalan and V. Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd., New Delhi 2010.
2. F.Basolo and R.G. Pearson, Mechanism of Inorganic Reaction, A Study of Metal Complexes in Solution, Wiley Eastern, New Delhi,1984.
3. J.E.Huheey, E.A.Keiter, R.L.Keiter and O.K.Medhi**,** Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, Pearson Education Inc., 2006.

Unit – IV

1. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, W.B. Saunders Company, 1977.
2. R.Gopalan and V. Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd., New Delhi 2010

Unit-V

1. K.F. Purcell and J.C. Kotz, Inorganic Chemistry, W.B. Saunders Company, 1977.

e- Resources

1. https://byjus.com/jee/coordination-compounds/
2. https://www.youtube.com/watch?v=8lT21wKoXyQ
3. https://byjus.com/chemistry/valence-bond-theory/
4. https://www.adichemistry.com/inorganic/cochem/reactionmechanism/transeffect/trans-effect-1.html
5. https://byjus.com/chemistry/organometallic-compounds/
6. https://www.youtube.com/watch?v=ITfwjQemwMg

PART III – CORE SUBJECT VI – PHYSICAL CHEMISTRY II

Hours per week: 5 **Credits: 4** **Subject Code: P22CHC23**

Course Outcomes:

On completion of the course, the students shall be able to

CO1: Will be in a position to discuss the need for approximation methods in quantum mechanics, basic concepts of chemical kinetics, catalysisand Group theory. [K2]

CO2: Will be able to predict antisymmetric nature of electron spin, various theories and their validity for the study of uni& bi-molecular reactions and the spectral selection rules of molecules with the aid of their symmetric properties. [K3]

CO3: Will be able to apply the concepts of Huckel molecularorbital calculations for the prediction of delocalization energies of π-electron systems, the study of reaction mechanism to fix the explosion limit of gas phase reactions and group theory for the theoretical prediction of hybridization in molecules [K3]

CO4: Can establish kinetics and mechanism for several branched and non-branched chain reaction and catalytic reactions and to construct the character tables using Great Orthogonality theorem.[K4]

CO5: Can develop applications of homogeneous, heterogeneous and enzyme catalytic reactions. [K5]

Unit I: Approximation methods in quantum mechanics **15 Hours**

Need for approximation methods -The Variation theorem; Linear Variation Principle, Perturbation theory. Applications of Variation Method and Perturbation Theory to the Helium atom – Hartree - Fock Self consistent field method - Electron spin, Anti symmetry and Pauli's exclusion principle – Slater determinant wave functions. Hund's rule and the term symbols of the electronic ground states of molecules - Born-Oppenheimer approximation, VB and MO theory, for H_2^+ molecular ion and H_2 molecule problems, Hückel Molecular Orbital theory and its application to ethylene, butadiene and benzene systems.

Unit II: Chemical kinetics I **15 Hours**

Brief resume of basic terms of chemical kinetics; Rate of a reaction, order & molecularity of a reaction, Empirical rate laws and units of rate and rate constants – influence of temperature on the rate of reaction – Arrhenius equation – Determination of activation energy of a reaction – Problems; Steady state approximation; Theories of reaction rates – Bimolecular collision theory and Absolute Reaction Rate Theory (ARRT); Theories of uni-molecular reactions – Lindemann's treatment – Rice, Ramsperger and Kassel (RRK) theory – The RRKM (Marcus) theory – Slater's theory; Reactions in solutions – influence of solvent dielectric constant, effect of ionic strength – Bronsted - Bjerrum equation – primary and secondary kinetic salt effect – effect of pressure on reaction rates – significance of volume of activation; Chain reactions and non-branched chain reactions – Kinetics and mechanism of H_2 - Br_2 reaction, Decomposition of CH_3CHO with order 3/2 and 1/2; Branched chain reactions; Explosion limits for gas phase reaction between H_2 and O_2.

Unit III: Catalysis **15 Hours**

Homogeneous catalysis – acid base catalysis – van't Hoff and Arrhenius intermediates for protolytic and prototropic mechanisms; Catalysis in Biological systems – enzyme catalysis – Michaelis – Menten kinetics – Line weaver and Burk plot – influence of pH on the enzyme catalysis; Heterogeneous catalysis – kinetics and mechanism of uni-molecular and bimolecular reactions – Langmuir-Hinshelwood and Langmuir - Rideal mechanism – ARRT of surface reactions.

Unit IV: Introduction to group theory **15 Hours**

Molecular symmetry elements and symmetry operations – various operations with illustrations; Groups and their basic properties – symmetry point group classification – rotational (C), dihedral (D), tetrahedral (Td) and octahedral (Oh) point groups; Order of a group - Classes and similarity transformation – Group multiplication table – cyclic and inverse rule – matrix representation of symmetry operations; Trace or character of the matrix – reducible and irreducible representations – Mulliken notation - Great orthogonality theorem – construction of character tables for C_{2v} and C_{3v} point groups.

Unit V: Application of group theory to solve spectroscopic and molecular problems **15 Hours**

Symmetry of normal modes of vibrations: linear ($C_{\infty v}$) and non-linear (C_{2v} and C_{3v}) molecules – physical basis of spectroscopic selection rules – properties of dipole moment, polarizability and definite integrals – IR and Raman active vibrational normal modes of homonuclear diatomic molecule (N_2) and heteronuclear diatomic linear molecules (CO and HCN) and non-linear molecules (H_2O, NH_3 & BF_3) – Mutual exclusion principle with illustration (CO_2 and XeF_4); Prediction of electronic transition and selection rules of organic compounds such as formaldehyde, ethylene and benzene; Group theoretical prediction of types of hybridization in CH_4, BF_3, $PtCl_4^{2-}$ and SF_6 systems.

TEXT BOOKS

1. A. K. Chandra, Introductory Quantum Chemistry, 3rdEdition, Tata-McGraw Hill Pub. Co., New Delhi, 1988.
2. K. J. Laidler, Chemical Kinetics, 3rdEdition, Pearson Education, 2007.
3. Ramakrishnan,V. & Gopinath, (2013).*Group Theory in Chemistry.* New Delhi: Vishal Publications, 2nd Edition.
4. Bajpai, D.N. (2011). *Advanced Physical Chemistry.* New Delhi**:** S.Chand & Co.,Ltd.,1st Edition.
5. Puri**,** B.R. Sharma .L. R and Pathania .M.S .(2003)**.** *Principles of Physical Chemistry.*New Delhi **:**Vishal Publishing Co**,** 1st Edition.

Reference books

1. D. A. McQuarrie, Quantum Chemistry, 1stIndian Edition, Viva Books (P) Ltd., New Delhi, 2003.
2. H.W. Hanna, Quantum Mechanics in Chemistry, Benjamin / Cummings Pub. Co., London, 1983.
3. I.N. Levine, Quantum Chemistry, 4thedition, Prentice-Hall India, New Delhi, 2000.
4. R.K. Prasad, (2000). *Quantum Chemistry*,New Delhi: New Age International publishers, 4thEdition.
5. E. House. (2008). *Fundamentals of Quantum Chemistry,*California: Academic Press, 2nd Edition.
6. D. A. McQuarrie and J.D. Simon, Physical Chemistry - A Molecular Approach, Viva Books (P) Ltd., New Delhi, 1998.
7. GurdeepRaj,S.(2003). *Advanced Physical Chemistry.*Meerut: Goel Publishing Co.25thEdition.
8. P.W. Atkins, and J.D. Paula, (2012). *Physical Chemistry.* New York: ELPS and Oxford University press, 7th Edition.
9. Raman, K.V. (1990)**.***Group Theory and Its Applications to Chemistry.* New York: Tata McGraw-Hill Publishing Company, 1st Edition
10. F. A. Cotton, Chemical Applications of Group Theory, 3rdEdition, John Wiley and Sons, New York, 1999.

11. Salahuddin Kunju, A., Krishnan, G. (2015).*Group Theory and Its Application in Chemistry.*Delhi: PHI Learning Pvt. Ltd., 3rd Edition.
12. G. Davison, Introduction to Group Theory for Chemist, Applied Sci., Pub., Ltd., London, 1971.
13. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders Co., London, 1977.

e - Resources:

1. https://youtube.com/channel/UCb1gintRG37w6-CAaGRm4Mg
2. https://youtube.com/playlist?list=PLOzRYVm0a65eW1kTGOrjBetXFMl4eaYVi- Quantum Mechanics
3. http://www.freebookcentre.net/Physics/Quantum-Mechanics-Books.html- Quantum Mechanics
4. https://drive.google.com/file/d/1zOzNV_gNlJLkXWtYee7PIe2V60Q12CDJ/view?usp=drivesdk – Basics of Chemical kinetics_pdf study material
5. https://youtube.com/playlist?list=PLxgQTTdYjh9pYy8abUUqDZibHbnDvJqbS - Chemical Kinetics
6. https://www.google.co.in/url?sa=t&source=web&rct=j&url=http://www.jiwaji.edu/pdf/ecourse/chemistry/Chemical%2520Kinetics.pdf&ved=2ahUKEwirhKvyv5z1AhUDsVYBHX5IA6g4ChAWegQIDxAB&usg=AOvVaw3AoZV_FpJBePZfCvOrX-tl – Chemical kinetics
7. https://www.google.co.in/url?sa=t&source=web&rct=j&url=http://mpbou.edu.in/slm/msccche1p4.pdf&ved=2ahUKEwiRrLLG4Zr1AhXSwosBHT46BDUQFnoECAMQAQ&usg=AOvVaw1Z7DbM1yusaSajeBkxqWNS– Symmetry & Group theory Study Material

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PART III– CORE I – LAB: ORGANIC CHEMISTRY PRACTICAL I

Hours per week: 3 **Credits: 3** **Subject Code: P22CHP21/** P19CHP21

Quantitative Analysis and Organic Preparations

Course Outcome:

CO 1: Over all, this practical skill is the basic principle and laid down the foundation for the synthesis and finding lead drug compounds for the treatment of several diseases in the world.

CO 2: Many macro molecules used as drug which can synthesis with help of simple molecule and principle.

CO 3: Also several textile industries dyeing the cloth with help of organic coloured compounds. The organic coloured compound can prepared with help of this fundamental preparations.

CO 4: Today's life can't survive without use of plastic. This practical skill can help to prepare plastic by polymerization of organic monomer.

CO 5: In order to prepare drug, pure form of drug is essential. The student can prepare the pure drug lead compounds and purification with help of chromatography skills.

1. Quantitative analysis:

(a) Estimation of glucose by Lane and Eynon method and Bertrand method.
(b) Estimation of glycine.
(c) Estimation of formalin.
(d) Estimation of Acetone.
(e) Estimation of unsaturation (cinnamic or maleic acid).
(f) Determination of equivalent weight of an acid.
(g) Chromatographic methods: Column, paper and TLC. (Class work only)

2. Organic preparations:

(a) *p*-bromoaniline from acetanilide
(b) *p*-nitroaniline from acetanilide
(c) m-nitrobenzoic acid from methyl benzoate
(d) benzilic acid from benzoin
(e) sym-tribromobenzene from aniline
(f) pinacolone from benzophenone (Photochemical reaction – class work only)
(g) anilide from benzophenone

PART III– CORE II – LAB: INORGANIC CHEMISTRY PRACTICAL I

Hours per week: 4 **Credits: 4** **Subject Code: P22CHP22/** P19CHP22

Course Outcome:

CO1: To study the basic idea behind the separation of cations.
CO2: To understand and execute the principles of inorganic qualitative and quantitative analysis.

Semi-micro qualitative analysis and complexometric titrations

Semi-micro qualitative analysis

Analysis of mixture containing two familiar and two less familiar cations from the following: W, Pb, Se, Te, Mo, Cu, Bi, Cd, Ce, Zr, V, Mn, Al, Ni, Co, Zn, Ba, Sr, Li and Mg. (Insoluble and interfering anions may be avoided).

Complexometric titrations

Estimation of one metal in the presence of another by EDTA

PART III– CORE III – LAB: PHYSICAL CHEMISTRY PRACTICAL I

Hours per week: 4 **Credits: 4** **Subject Code: P22CHP23/** P19CHP23

Course Outcome:

CO1: Will be in a position to apply the theoretical concepts of electrochemistry, partition coefficients, chemical kinetics, surface chemistry and spectroscopy by the way of performing simple experiments.
CO2: Will be able to extend the applications of potentiometric and conductometric techniques to find out dissociation constant of weak electrolytes, pH of solutions and solubility of sparingly soluble salts.
CO3: Can calculate various physical constants by the way of performing experiments.
CO4: Will be able to interpret the UV Visible and IR spectra and spectrofluorometric data of simple compounds.
CO5: Can establish the applications of various techniques learnt for designing projects.

I. Conductometric experiments

(i) Double displacement and acid base titrations
(a) $NH_4Cl \rightarrow NaOH \rightarrow$ Mixture of CH_3COOH and HCl
(b) $NH_4Cl \rightarrow NaOH \rightarrow$ Mixture of NH_4Cl and HCl

(ii) Precipitation titrations
(a) $Na_2CO_3 \rightarrow Pb(NO_3)_2 \rightarrow Na_2CO_3$
(b) $K_2SO_4 \rightarrow BaCl_2 \rightarrow K_2SO_4$

(iii) Determination of cell constant of a conductivity cell, pH and dissociation constant of weak acids.

II. Distribution experiments

(i) Distribution of iodine between CCl_4 and H_2O

(a) Determination of partition coefficient
(b) Determination of equilibrium constant of the reaction $KI + I_2 \rightarrow KI_3$
(c) Determination of concentration of given KI solution by distribution method.

(ii) Distribution of benzoic acid between water and benzene

III. Kinetic Experiments

Kinetic study of the reaction between $K_2S_2O_8$ and KI – second order reaction under equimolar concentration.

IV. Adsorption Experiments

1. Adsorption of oxalic acid on charcoal
2. Adsorption of acetic acid on charcoal

V. Potentiometric methods

1. Precipitation titration: Ag^+ *vs* halide mixture
2. Redox titrations: a) permanganate *vs* iodide ion
   b) dichromate *vs* ferrous ion.
3. Determination of dissociation constant of weak acids
4. Determination of pH of buffer solutions
5. Determination of solubility product of sparingly soluble salts.

VI. Titrations using pH meter (Class work only)

Determination of first, second and third dissociation constants of phosphoric acid.

VII. Experiments based on UV-Visible, Infrared spectrophotometers and spectrofluorometer. (Class work only)

*Field/Industrial visit (Report submission only)

PART IV – NON-MAJOR ELECTIVE – INDUSTRIAL CHEMISTRY

Hours per week: 4 **Credits: 4** **Subject Code: P22CHN21**

COURSE OUTCOMES

On completion of the course, the students shall be able

CO1: The role of chemistry industry.
CO2: Gain the knowledge / processes of various industries.
CO3: Understand the principles of Soap/polymer/Oil industries.
CO4: Get exposure of importance of chemistry industry.
CO5: Gain the processes involved in small / large scale chemistry industries.

Unit I: Importance of chemical process industry 12 Hours

Introduction– origin and development of chemical process industry – pre-scientific chemical industry – scientific chemical industry. Growth with restraints – Green challenge to chemical industry – Indian chemical industry today – classification of technologies processes – basic principles of homogeneous and heterogeneous processes.

Unit II: Energy for chemical industry 12 Hours

Fuels – definition - characteristics of a good fuel-classification of fuels-fossil fuel – Types of fossil fuel - solid, liquid, gaseous fuels – coal-origin and chemical composition – classification of coals – calorific value – Types of gaseous fuel -Natural gas –Oil gas – Cracking - Producer gas – Coal gas – Water gas – Gobar / biogas –Fischer – Tropsch process.

Unit III: Water conditioning in chemical process industry **12 Hours**

Introduction – sources of water supply – characteristics of water – water for industrial purpose – Types of water - soft and hard water – softening of water – Permutit process – ion exchange process. Types of hardness – disadvantages of using hard water in industry – Desalination of water – Reverse osmosis process.

Unit IV: Small scale chemical industry **12 Hours**

Oils and fats – composition of oils – Difference between oils and fats – paraffin waxes – candles – Soaps - Types and manufacture of soaps by continuous process.Polymers – Types of polymerization – Addition, copolymerization – condensation classification of polymers – Plastics –Thermoplastic -Thermosetting – PVC – Teflon – Terylene – natural rubber – synthetic rubber

Unit V: Large scale chemical industry **12 Hours**

Portland cement – Raw materials – Manufacture of cement - composition of cement – role of gypsum – setting of cement – fertilizer – classification of fertilizers – indirect and direct fertilizers – Nitrogenous fertilizer Urea – Raw materials required for preparation of urea and production process of urea - NPK fertilizers & their advantages – Industrial effluents and treatment

Reference Books

1. O. P. Vermani, A. K. Narula, Industrial Chemistry, 2004, Galgotia Publications, New Delhi.
2. W.V.Mark, Chemical Process Industries, Vol. I and II, 2nd edition, CBS Publication, S.C.Bhatia, 2008.
3. AllaAppa Rao, Engineering Chemistry and Environmental Studies, New AgeInternationalPublishers, 1st edition, 2010.
4. Mukhyonov (ed), Chemical Technology Vol.I, MIR Publication, Moscow, 3rd edition,1979.
5. B.N.Chakrabarthy, Industrial Chemistry, Oxford and LBH Publ., New Delhi, 1984.
6. B.K.Sharma, Industrial Chemistry, Goel Publishing House, 6th edition, 1994.

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1. https://www.sciencedirect.com/topics/social-sciences/small-scale-industries
2. https://shodhgangotri.inflibnet.ac.in/bitstream/123456789/271/2/02_introduction.pdf
3. https://www.ibef.org/industry.aspx
4. https://niti.gov.in/planningcommission.gov.in/docs/plans/planrel/fiveyr/7th/vol2/7v2ch4.html
5. https://chem.libretexts.org/Bookshelves/Analytical_Chemistry/Supplemental_Modules_(Analytical_Chemistry)/Electrochemistry/Electrolytic_Cells/Electroplating

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Course Name: Master of Science
Discipline: Chemistry
CHOICE BASED CREDIT SYSTEM
(For those who joined in June 2018 and after)
Course scheme:

Semester	SUBJECT	Hours	Credit	Int+Ext= Total	Local	Regional	National	Global	Professional Ethics	Gender	Human Values	Environment & Sustainability	Employability	Entrepreneurship	Skill Development	Subject code	Revised / New / No Change / Interchanged & Percentage of revision
III	Core Subject VII-Organic Chemistry III	5	4	40+60=100				✔	✓							P19CHC31	Revised / 25 %
	Core Subject VIII-Inorganic Chemistry III	5	4	40+60=100				✔	✓							P19CHC32	Revised / 5 %
	Core subject IX-Physical Chemistry III	5	4	40+60=100				✔	✓							P19CHC33	Revised / 1 %
	Core Lab IV-LAB: Organic Chemistry Practical II	4	-	-				✔	✓							-	No Change
	Core Lab V-LAB: Inorganic Chemistry Practical II	4	-	-				✔	✓							-	No Change
	Core subject X - Analytical Methods in Chemistry	3	3	40+60=100				✔	✓							P19CHC34	No Change
	Major Elective 2- Medicinal and Pharmaceutical Chemistry / Polymer Chemistry	4	4	40+60=100				✔	✓							P19CHE31/ P19CHE32	No Change
IV	Core subject XI-Organic Chemistry IV	5	4	40+60=100				✔	✓							P19CHC41	Revised / 20 %
	Core subject XII-Inorganic Chemistry IV	5	4	40+60=100				✔	✓							P19CHC42	Revised / 2 %
	Core subject XIII-Physical Chemistry IV	5	4	40+60=100				✔	✓							P19CHC43	No change
	Core Lab IV-LAB: Organic Chemistry Practical II	4	4	40+60=100				✔	✓							P19CHP41	No change
	Core Lab V-LAB: Inorganic Chemistry Practical II	5	5	40+60=100				✔	✓							P19CHP42	No change
	Major Elective 3: Project & Viva-voce	6	5	40+60=100				✔	✓							P19CH4PV	No change

Self-Learning Courses:

Year	Semester	Subject	Credit	Ext =Tot	Subject Code
II	III	Applied Chemistry	5	100 = 100	P19CHSL31
II	III	CRITICAL ANALYSIS OF GATE/CSIR-NET QUESTIONS	5	100 = 100	P19CHSL32

Semester - III Core Subject VII - Organic Chemistry III

Hours per week: 5 **Credits: 4**

Subject Code: P19CHC31

Objectives:

- To plan and execute organic synthesis
- To get mastery over photochemical, oxidation, reduction and rearrangement reactions.
- To study the structural elucidation of heterocycles,
- To revise the structure of carbohydrate.

Unit I: Synthetic methods I **(15 hours)**

Introduction to Organic synthesis- C-C bond forming reaction –functional group modification – 1,2-carbonyl addition- 1,4-carbonyl addition- nucleophilic addition to carbonyl compounds and olefin)-synthetic methods – Planning a synthesis – molecular history- Relay approach-starting material-Activating groups-protecting groups - molecular size –convergent approach-carbon skeletal complexity (Robinson annulation, Michael addition, Diel-Alder reaction)-functionality, steric crowding – Stereo selective problems of geometrical and optical isomerism (problems associated with optical isomerism- control of asymmetry-separation of optical isomers)- -transition metal complexes in organic chemistry.

Reference books :

1. R.E.Ireland, Organic synthesis, Prentice – Hall of India Pvt. Ltd., 1975.
2. R.T.Morrison and R.N.Boyd, Organic Chemistry, Prentice – Hall of India, New Delhi, 6th Edn., 1995.
3. M.B.Smith, Organic Synthesis, McGraw-Hill, International Edn., New Delhi, 1994.
4. W.Carruthers and Iain Coldhain, Modern Methods in Organic Synthesis, 4th Edn., Cambridge University Press, U.K., 2008
5. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part B, V Edn., Springer, New York, 2007.
6 R.O.C.Norman, Principles of Organic Synthesis, Methuen & co Ltd, 1968.
7. I.L.Finar, Organic chemistry,Vol.II, English Language Book Society,1977.
8. S.Murugan, Organic Synthesis-An Introduction

Unit II: Organic photochemistry and pericyclic reactions **(15 hours)**

Organic photochemistry: Basic principle (Thermal versus photochemical reaction, photochemical laws – electronic excitation – allowed and forbidden transition – internal conversion and inter system crossing – Jablonski diagram) – Photochemical reactions (primary and secondary step) – photosensitization- photochemistry of olefins (dimerization – *cis-trans-*

isomerisation) – photochemical reactions of ketones (Norrish type I and Norrish type II reactions) –Paterno-Buchi reaction – Photo-oxidation and photo reduction – Di-π-methane rearrangement.

Pericyclic reaction: Conservation of orbital symmetry-construction of molecular orbital and symmetry elements to simple molecules like 1,3-butadiene, 1,3,5-hexatriene, cyclobutene, cyclohexadiene- Electrocyclic reactions – Cycloaddition reactions- Sigmatropic rearrangement reactions – Application of FMO approach – Correlation approach – Huckel-Mobius approach-(dis- and con- rotatory ring closure of 1,3-butadiene, 1,3,5-hexatriene and (2 π + 2 π),(4 π + 2 π) cycloaddition reaction).

Reference books :

1. C.H.Depuy and O.L.Chapman,Molecular reactions and Photochemistry, Prentice Hall, New York, 1988.
2. A.J.Bellamy, An Introduction to conservation of orbital symmetry, Longman, 1974.
3. S.M.Mukherji and S.P.Singh, Reaction Mechanism in Organic Chemistry, McMilan India Ltd., 1978.
4. R.B.Woodward and R.Hoffmann, The Conversion of Orbital Symmetry, Verlog Chemie Gmbh and academic press, 1971.

Unit III: Molecular rearrangement (15 hours)

Mechanism of the following rearrangement reactions – Carbon to carbon migration (Wagner-Meerwein, Demzanov, Wolff and dienone-phenol rearrangement)-Carbon to nitrogen migration (Curtius, Schmidt and Lossen rearrangement) - Carbon to oxygen migration (Bayer-Villiger, Favorskii rearrangement)- Rearrangement proceeding through carbanions (Stevens, Sommelet-Hauser and Shapiro rearrangement). Free radical reactions –Barton, Sand Meyer, Gomberg, Ullmann, Pschorr and Hundsdiecker reaction.

Reference books :

1. R.B. Woodward and R. Hoffmann, The Conversion of Orbital Symmetry, Verlog Chemie Gmbh and Academic Press , 1971.
2. H.H. Jaffe and M. Orchin, The Importance Antibonding Orbitals, Oxford and IBH, 1967.
3. A.J. Bellamy, An Introduction to Conservation of Orbital Symmetry, Longman, 1974.
4. J. March, Advanced Organic Chemistry, John Wiley & sons, 4th Edn., New York , 1992.
5. I.L. Finar, Organic Chemistry , Vol. II , 5th Edn., Pearson Education Ltd., New Delhi, 2011.
6. P.De.Mayo, Molecular Rearrangement.

Unit IV: Heterocyclic compounds and Carbohydrates (15 hours)

Heterocyclic compounds: Nomenclature of heterocycles having not more than two hetero atoms-Structure, synthesis and reactions of Oxazole, Imidazole, Thiazole, Coumarin, Flavone and Flavanol (3-hydroxyflavone), Anthocyanins (Quercetin, Cyanin, Cyanidin chloride) –

Pyrimidines (Uracil) and Purines (Structural elucidations of Caffeine, Theobromine and Theophylline).

Carbohydrates: Ring structure of the monosaccharides – Methods for determining the size of sugar rings – Chemistry, configuration and conformation of lactose and cellobiose – Chemistry of starch and cellulose.

Reference books :

1. R.M.Achesan, Chemistry of Heterocyclic Compounds, Wiley Eastern, 1973.
2. I.L.Finar, Vol.II, 5th Edn., Pearson Education Ltd., New Delhi, 2011.
3. Joule and Smith, Heterocyclic Chemistry 4th Edition Black Well Publishers, 2000.
4. Raj K.Bansal, Hereocyclic chemistry, Wiley Eastern Limited, New Delhi, 1990.
5. S.F.Dyke, Chemistry of Carbohydrates, Interscience Publishers Ltd., London, 1960.
5. J.L.Jain, Fundamental of Biochemistry, 4th Edn., S.Chand & Company Ltd., New Delhi, 1998.
6. A.L.Lehninger, Principles of Biochemistry, W.H.Freeman and company, New York, 2005.

Unit V: Oxidation and reduction (15 hours)

Reaction mechanism, application and stereochemical aspects of the following Oxidation and Reduction reactions – Oxidation reactions involving CrO_3, SeO_2, OsO_4, lead tetraacetate, periodic acid, NBS, H_2O_2 – Oppenauer oxidation.

Reduction involving catalytic hydrogenation, electron transfer, hydride transfer ($LiAlH_4$, and $NaBH_4$) reduction, DIBAL(diisobutylaluminium hydride), triisobutoxyalumino hydride, - Selectivity in oxidation and reduction - Hydroboration- Birch reduction –MPV reduction- Wolff Kishner reduction – Hauang – Minlon reduction.

Reagents in Organic synthesis – Gilman's reagent (lithium dimethylcuprate) - LDA (lithium diisopropylamide), DCC (dicyclohexylcarbodiimide), DDQ (2,3-dichloro-5,6-dicyanobenzoquinone), 1,3-dithiane (Umpolung synthesis), Woodward and Prevost hydroxylation, Baker yeast- Phase transfer catalyst.

Reference books :

1. R.O.C.Norman, Organic Synthesis, 3rd Edn., 1993.

2. W.Carruhers and Iain Coldhain, Modern Methods in Organic Synthesis, 4th Edn., Cambridge University Press, U.K., 2008.

3. S.HPine, J.B.Herndrickson, D.J.Cram and G.S.Hammond, Organic Chemistry, McGraw Hill Kogakusha Ltd., Tokyo, 4th Edn., 1980.

4. H.O.House., Modern Synthetic Reactions, W.A.Benjamin Inc. California, 2nd Edn., 1972.

5. P.S. Kalsi, Organic reactions and their Mechanisms, New Age International(P) Limited,Publishers,2nd Edn., 2007.

Semester III – Part III – Core Subject VIII – Inorganic Chemistry III

Hours per week: 5 **Credits: 4**

Subject Code: P19CHC32

Objectives:

- To understand the importance of various bio-inorganic compounds.
- To study the role of inorganic chemistry in biological system.
- To be well-versed in electronic spectra, NMR, EPR and Mossbauer spectra of inorganic compounds.

Unit I – Bioinorganic Chemistry I **(15 hours)**

Porphyrin ring system – metalloporphyrins – cytochrome-C – dioxygen binding transport and utilization - hemoglobin and myoglobin – structure and work function – Synthetic oxygen carrier - physiology of blood - Chlorophyll – structure – photosynthetic sequence – Corrin ring system – Vitamin B_{12} and Vitamin B_{12} coenzymes – *in vivo* and *in vitro* Nitrogen fixation.

Essential and trace elements in biological system – Molecular mechanism of ion transport across membrane – natural and synthetic ionophores – sodium - potassium ion pump.

Unit-II - Bioinorganic Chemistry II **(15 hours)**

Metalloenzymes– superoxide dismutase, peroxidases and catalases. Zinc enzymes – structure and function - Carboxypeptidase A – Carbonic anhydrase and Alcohol dehydrogenase – structural role of zinc and zinc constellations.

Non-heme iron proteins – iron-sulphur proteins – Copper containing proteins – classification – blue copper protein – structure and function.

Chelate therapy – detoxification of metal poisoning in functional groups of enzyme – anticancer activity of cis-platin – interactions of cis-platin with DNA. Gold compounds as anti-arthritic agents - Metals in radiodiagnosis and MRI.

Reference books (Units I & II)

1. K.Hussain Reddy Bioinorganic Chemistry, New Age Publishers, New Delhi, (2009).
2. J.E. Huheey, E.A. Keiter and R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity (4th edition): Pearson Education Inc.,2006.
3. L.Stryer, Biochemistry, IV Edn., Freemann and Company, New York (1995).
4. D.L Nelson & M.M.Cox, Lehninger Principles of Biochemistry , 5th edition Freemann and Company, New York (2011).

Unit III –Electronic Spectra **(15 hours)**

LS coupling – Term symbols for ground and excited state – d-d transition – Charge transfer transition – selection rules – mechanism of breakdown of selection rules – bandwidths and shapes – Orgel diagram – Tanabe-Sugano diagram – Electronic spectra of transition metal complexes - Jahn-Teller effect – evaluation of 10Dq and β for octahedral complexes of d^2, d^3, d^6, d^7 and d^8 configurations.

Reference books

1. J.E. Huheey, E.A. Keiter and R.L. Keiter, Inorganic Chemistry Principles of Structure andReactivity (4th edition): Pearson Education Inc.,2006.

2. F.A.Cotton and G.Wilkinson, Advanced Inorganic Chemistry (6th edition), JohnWiley&Sons, New York, 2006.
3. J.D. Lee, Concise Inorganic Chemistry , 5th edition, Blackwell Science, 2000.
4. D.F.Shriver, P.W.Atkins and C.H.Langford, Inorganic Chemistry, 3rd edition, Oxford Univ.Press, 1999.
5. R.S. Drago, Physical Methods in Inorganic Chemistry , Van Nostrand Reinhold Co., New York (1965).
6. D.N.Sathyanarayana, Electronic Spectroscopy and Related Techniques, Universities Press Limited (2001).

Unit IV–EPR Spectroscopy of Inorganic Compounds (15 hours)

Principle of EPR – presentation of the spectrum – hyperfine splitting – g value – isotropy and anisotropy in g value – factors affecting the magnitude of g values – zero field splitting – Kramer's degeneracy – anisotropy and hyperfine splitting constant – Application of EPR in transition metal complexes VO^{2+} Fe^{3+} Co^{2+} ,Mn^{2+} and bis-salicylaldimine copper (II) – Covalency of metal complexes (Copper) - Jahn-Teller distortion studies in Cu(II) complexes .

Fundamentals of ENDOR techniques.

Unit V – NMR and Mossbauer Spectroscopy (15 hours)

NMR : Introduction – applications of ^{31}P, ^{19}F and ^{15}N - NMR spectroscopy used in structural problem – evaluation of rate constants – NMR of fluxional molecules – NMR of paramagnetic molecules – contact shifts and Pseudo contact shift and Lanthanide shift reagents.

Mossbauer spectroscopy: Mossbauer effect resonance absorption – Doppler effect Doppler velocity – Experimental technique of measuring resonance absorption – isomer shift – effect of quadruple nucleus – magnetic hyperfine splitting – Applications of Mossbauer spectroscopy in the study of iron, gold and tin complexes.

Reference books (Unit IV & V)

1. R.S. Drago, Physical Methods in Inorganic Chemistry , Van Nostrand Reinhold Co., New York (1965).
2. Atkins, Overton. Inorganic chemistry-IV edn
3. E.B.A. Ebsworth, D.W.H. Ranklin and S. Gadock Structural Methods in Inorganic Chemistry, ELBS Edn., (1988).
4. R. L. Dutta and A. Syammal, Elements of Magnetochemistry, 2nd edition, EWP Pvt. Ltd., New Delhi (1993).

Semester - III - Part – III - Core Subject IX - Physical Chemistry III

Hours per week: 5 **Credits: 4**

Subject Code: P19CHC33

Objectives:

- To study electrochemistry in detail.
- To make students in competent to microwave, infra-red and electronic spectra.
- To perceive statistical thermodynamics.

Unit I: Electrochemistry I (15 hours)

Conductivities of ions- conductance of strong and weak electrolytes- Determination of equivalent conductance of weak electrolyte at infinite dilution- Kohlrausch's law and its applications- Theory of electrolytic conductance- inter-ionic attraction- ionic atmosphere - thickness of ionic atmosphere- Debye-Huckel-Onsager equation- its derivation and experimental

verification- deviations and modifications- Debye Falkenhagen and Wein effects – mean ionic activity and activity coefficients of strong electrolytes- Debye- Huckel limiting law- Applications of conductance measurements- Determination of solubility of sparingly soluble electrolytes- Determination of dissociation constant of weak acids - conductometric titrations.

Unit II: Electrochemistry II **(15 hours)**

The role of electrodes - electrochemical potential- Types of electrodes- the gas/inert metal electrode- ion / insoluble salt / metal electrode- oxidation-reduction electrode liquid junction potential and membrane potential – Electrochemical cells- kinds of cells notation- electrochemical cell reactions – EMF of cells- Nernst equation- Application of EMF measurements- determination of equilibrium constant, dissociation constant, solubility product and potentiometric titrations.

Types of overpotential- Effect of overpotential on the rate of electro-chemical reactions - Butler-Volmer equation - Tafel equation - Current potential curves - Hydrogen over voltage - Application of electrochemical processes- power generation and storage- Fuel cells- storage batteries and dry cells.

Reference books : (unit I & II)

1. D.R. Crow, "Principles and Application of Electrochemistry", Chapmann Hall, London (1988).
2. J.O.M. Bockris and A.K.N. Reddy, "Modern Electrochemistry" Vol. I & II, Plenum Press, New York (1970).
3. L.Antropov, "Theoretical Electrochemistry" Mir Publications, Moscow (1972)
4. S.Glasstone, An Introduction to Electrochemistry.
5. B.Viswanathan, S. Sundaram, R. Venkataraman, K. Rengarajan and P.S. Raghavan, "Electrochemistry-Principles and Applications" S. Viswanathan Printers and Publishers Pvt., Ltd., (2007)

Unit III: **Statistical Thermodynamics** **(15 hours)**

Definition of state of a system- ensembles (micro, macro and grand canonical) - Boltzmann distribution law and its derivation- Boltzmann- Planck equation- partition functions - thermodynamic properties from partition functions - partition function and equilibrium constant- Quantum statistics - Fermi-Dirac and Bose- Einstein statistics- photon gas and electron gas according to such statistics- population inversion- Einstein's and Debye's theories of heat capacities of solids. Nuclear spin statistics - statistical basis of entropy of H_2 gas - ortho and para nuclear states- calculation of residual entropy of H_2 at 0 K in terms of ortho-para ratio-Sackur-Tetrode equation

Reference books :

1. J. Rajaram and J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Applications of Femtochemistry, Macmillan India Ltd., (2008).
2. H.K. Moudgil, Textbook of Physical Chemistry, PHI Learning Pvt., Ltd., New Delhi (2010).
3. D.A. McQuarrie and J. D. Simon, Molecular Thermodynamics, Viva Books Pvt., Ltd., New Delhi (2004).
4. F.W. Sears and G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics" 3rd Edn., Narosa Publshing House, New Delhi (1991).

5. B.R. Puri, L.R. Sharma and M.S. Pathania, Principles of Physical Chemistry (Millennium Edn,) Vishal Publishing Co., (2003)
6. J. Kestin and J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, New York (1971).
7. R.P.H. Gasser, W.G. Richards, Entropy and Energy Levels, ELBS Edn., Oxford University Press (1974).
8. B.R. Puri, L.R. Sharma and M.S. Pathania, Principles of Physical Chemistry (Millennium Edn,) Vishal Publishing Co., (2003)

Unit IV – Molecular Spectroscopy I (15 hours)

Microwave spectroscopy- rotational classes of molecules - rotational spectra of rigid diatomic molecules- effect of isotopic substitution- relative intensity of rotational spectral lines- Stark effect in microwave spectra - Information derived from rotational spectra.

Infrared spectroscopy- energy of a diatomic molecule based on harmonic and anharmonic oscillator model- selection rules- diatomic vibrating rotator - vibrations of polyatomic molecules- fundamental vibrations and their symmetry with illustration (H_2O and CO_2) - overtone, hot bands combination and difference bands - influence of rotation on the spectra of polyatomic molecules - concept of group frequencies - Fermi resonance- Fourier transform infrared spectroscopy.

Unit V: Molecular spectroscopy II (15 hours)

Raman spectroscopy- Quantum and classical theories of Raman scattering- Rotational Raman spectra of diatomic molecules- rotation-vibration Raman spectrum- Mutual exclusion principle- Laser Raman spectroscopy.

Electronic spectra of diatomic and polyatomic molecules- intensity of vibrational electronic spectra - Franck-Condon principle- rotational fine structure of electronic vibrational spectra- the Fortrat parabola- Dissociation and predissociation spectra.

Reference books : (unit IV & V)

1. C.N.Banwell and E.M.McCash, Molecular Spectroscopy, Tata McGraw Hill, 4th Edn., (1995).
2. G. Aruldhas, "Molecular Structure and Spectroscopy", 2nd Edn., Prentice-Hall of India Pvt., Ltd., New Delhi (2007).
3. R.S.Drago, Physical Methods in Chemistry, W.B. Saunders Co., London (1977).
4. D.C. Harris and M.D. Bertolucci, Symmetry and Spectroscopy-An Introduction to Vibrational and Electronic Spectroscopy, Oxford University Press, New York (1978).
5. G.H.Barrow, Introduction to Molecular Spectroscopy, McGrawHill.
6. R.Chang, Basic Principles of Spectroscopy, McGraw Hill, London (1976).
7. B.F. Straughan and S. Walker (eds.), Spectroscopy, Vol. 1, 2 and 3, Chapman & Hall, London (1976).

Semester - III - Part – III – Core Subject X
Analytical Methods in Chemistry

Hours per week: 3 **Credits: 3**
Subject Code: P19CHC34

Objectives:

- To provide basic understanding of electroanalytical and thermoanalytical techniques.
- To study the importance of various spectroanalytical methods.

Unit – I Thermoanalytical Methods (9 hours)

Thermogravimetic analysis (TGA) – principle – instrumentation – factors influencing the thermogram – applications of TGA – derivative thermogravimetry. Differential thermal analysis (DTA) – principle – instrumentation – applications of DTA – comparison of TGA and DTA thermogram. Differential Scanning Colorimetry – principle and applications. Thermometric titrations – apparatus – applications.

Unit – II Electroanalytical Methods – I (9 hours)

Theory of electrogravimetric analysis – types- constant current electrolysis – constant potential electrolysis - electrolytic separation and determination of metal ions – Coulometry – principle- types of coulometric analysis – coulometric titration and its applications – constant potential coulometry and its applications.

Unit – III Electroanalytical Methods – II (9 hours)

Voltammetry – current voltage relationship – cyclic voltammetry – electrodes used in cyclic voltammetry – applications of cyclic voltammetry. Polarography – principle – dropping mercury electrode – experimental technique – polarographic curves – applications to qualitative and quantitative analysis. Theory of chronopotentiometry. Amperometric titrations – principle – apparatus used – applications – advantages and disadvantages. Stripping analysis.

Unit – IV Spectroanalytical Methods – I (9 hours)

Optical rotatory dispersion (ORD) and circular dichroism (CD) phenomenon – ORD and CD for the study of metal complexes.

Photoelectron spectroscopy – principle – spectra of diatomic molecules – spectra of N_2, O_2, F_2 and CO – effect of spin orbit coupling – spectra of poly atomic molecules (H_2O, NH_3, CH_4, VCl_4, $TiCl_4$, and $Ni(CO)_4$.

Auger electron spectroscopy – principles and applications.

Unit – V Spectroanalytical Methods – II (9 hours)

Spectrofluorometry – principle – instrumentation – applications of spectrofluorometry. Flame photometry – principle, instrumentation and applications. Atomic absorption spectroscopy - principle, instrumentation and applications. Principle and instrumentation and applications of nepheleometry and turbidimetry. Determination of sulphate and phosphate.

References books:

1. H.H. Willard, L.L.Merritt and J.A. Dean, Instrumental Methods of Analysis, 7th edition, Wadsworth Publishing Company, USA (1986).
2. D.A.Skoog and D.M.West, Principles of Instrumental Methods of Analysis, 2nd edition, Saunders Publishers, New York, (1980).

3. D.A. Skoog, D.M. West and F.J. Hollar, Fundamentals of Analytical Chemistry, 7th Edition, Harcourt College Publishers, 1996
4. J.G,Dick, Analytical Chemistry, Tata-McGraw Hill, New Delhi(1973).
5. J. Basset et al., Vogel`s Text book of Qualitative Inorganic Analysis, Longman, 5th Edition, ELBS, Essex, 1989.
6. D.N.Sathyanarayana, Electronic Spectroscopy and Related Techniques, Universities Press Limited (2001).

Semester - III - Part – III – Major Elective III
Medicinal and Pharmaceutical Chemistry

Hours per week: 4 **Credits: 4**
Subject Code: P19CHE31

Objectives:

- To get mastery over all the fundamentals of medicinal chemistry.
- To study the synthesis, mechanism, action and applications of various types of drugs.

Unit I: Fundamentals of Medicinal Chemistry (12 hours)

Definitions of Medicinal Chemistry, Pharmacology, Pharmacodynamics, Pharmacognosy, drugs – Nature and sources of drugs, routes of administration of drugs – General principle of drug action – drug action at active sites – biotransformations of drug – factors affecting the drug action – catalytic role of enzymes.

Receptor – Drugs – receptor bonding, Drug action at receptor – theories of receptor – QSAR – Hansch approach, Craig plot – bioisosteres.

Reference Book

1. An Introduction to Medicinal Chemistry, Graham L. Patrick, Oxford University Press, 1995.

Unit II: Prodrugs, Agonist & medicinally useful antibiotics and hormones (12 hours)

Prodrugs, classification, design, bioprecursor and application. Structural features and mode of action of β-lactum antibiotics. agonist, design of agonist and its requirements-antagonist, design of antagonist – partial agonist. Biosynthesis of insulin and thyroid hormones

Reference Book

1. Text book of Medicinal Chemistry, Volumes I & II, K. Ilango and P.Valentina, Keerthi Publishers, 2007.

Unit III: A few important Chemotherapeutic Agents. (12 hours)

Antineoplastic Agents: Classification, synthesis and assay eg: Chlorambucil, Busulfan, Methotrexate, 5-Flurouracil, Ifosfamide, and Cis-platin

Antitubercular drugs: Classification, synthesis and assay eg: Isoniazid, Rifampicin(assay only), Ethionamide, Pyrazinamide, Thiacetazone and *p*-Aminosalicylic acid.
Antimalarial drugs: Classification, synthesis and assay eg: Chloroquine, Mefloquine, Proquanil, Pyrimethamine and Amodiaquine

Unit IV: Synthesis, mechanism of action and uses of antihypertensive, antiviral and diuretics drugs. (12 hours)

Antihypertensive drugs: Methyldopa, Hydralazine, Propranolol, Nifedipine and Captopril.
Antiviral drugs: Acyclovir, Methisazone, Amantadine, Didanosine and Delavirdine
Diuretics: Furosemide, Acetazolamide and Chlorothiazide

Unit V: Synthesis, SAR and therapeutic uses of anti-inflammatory and CNS drugs. (12 hours)

Anti-inflammatory drugs: Aspirin, Paracetamol, Phenylbutazone, Ibuprofen and Mefenamic Acid
CNS - Stimulant drugs: Amphetamine, Caffeine, Theobromine, Theophylline and Nikethamide.
CNS - depressant drugs: Phenelzine, Imipramine, Desipramine, Nortiptyline and Amitriptyline.

Reference Books: (unit III, IV & V)

1. Medicinal Chemistry, D.Sriram and P.Yogeeswari, Pearson Education publishers, 2007.
2. Medicinal Chemistry, G.R.Chatwal, Himalaya Publishing House, 2002
3. A text book of Pharmaceutical Chemistry, Jeyashree Ghosh, S.Chand Publishers 2012.
4. Medicinal Chemistry, Ashutosh Kar, New Age International Publishers, 2007.
5. https://www.pharmacopoeia.com/

Semester - III - Part – III – Major Elective III
Polymer chemistry

Hours per week: 4 **Credits: 4**
Subject Code: P19CHE32

Objectives:
- To study the classifications and properties of different polymers
- To learn the various polymerization techniques.

Unit I: Classification of polymers and chemistry of polymerization (9 hours)

Classification of polymers: Linear polymers, non-linear or branched polymers, cross – linked polymers, homo chain and hetero chain, homopolymers, co-polymers, block polymers and graft polymers.

Chemistry of polymerization: Types of polymerization – mechanism – chain, growth, free radical, ionic, co-ordination, ring opening, group transfer, polyaddition and polycondensation polymerizations.

Unit II: Individual polymers (9 hours)

Monomers required for general methods of preparation, repeat units and uses of the following polymers and resins – polyethylene, polystyrene, polyacrylonitrile, polymethylacrylate, PVC, polytetrafluoroethylene, polyisoprenes, polybutadienes and polychloroprene, polyesters, polycarbonates, polyimides, polyamides (Kelvar), polyurethanes, polyethylene glycols, phenol-formaldehyde, urea-formaldehyde, melamine formaldehyde and epoxy resins – silicone polymers.

Reference books : (unit I & II)

1. V.R.Gowariker, N.V.Viswanathan and Jayadev Sreedhar, "Polymer Science", Wiley Eastern Ltd., New Delhi, 1986.
2.G.Odian, "Principles of Polymerization", 2nd edn., John Wiley and Sons, New York, 1981.
3. B.K.Sharma, "Polymer Chemistry", Goel Publishing House, Meerut, 1989.
4. P.J.Flory, "Principles of Polymer Chemistry", Cornell Uni. Press, Ithaca, 1953.

Unit III: Properties of polymers (9 hours)

Intrinsic properties – processing properties – article properties – basic idea of isomerism of polymers – configuration of polymer chain – geometrical structure – syndiotatic, isotatic and atatic polymers.

Glass transition temperature – Definition – factors affecting glass transition temperature – relationships between glass transition temperature and (a) molecular weight, (b) melting point and (c) plasticizer – importance of glass transition temperature – heat distortion temperature.

Molecular weight and size of polymers: Number average, weight average, sedimentation and viscosity average molecular weights – molecular weights and degree of polymerization – poly dispersity – molecular weight distribution in polymers – size of polymer molecules – kinetics of polymerization.

Reference book :

1. D.W.van Krevelen and P.J.Hoftyrager, "Properties of Polymers", Elsevier, New York, 1976.

Unit IV: Polymerization techniques, degradation and uses of polymers (9 hours)

Polymerization techniques: Bulk, solution, suspension, emulsion, melt condensation and interfacial polycondensation polymerizations.

Degradation: Types of degradation – thermal, mechanical, ultrasonic and photo degradation – photostabilizers – oxidative degradation – antioxidants – hydrolytic degradation. Uses of polymers in electronics and biomedicine.

Reference books :

1. F.W.Billmeyer, "Textbook of Polymer Science", 3rd edn., John Wiley and Sons, New Your, 1984.
2. Harry R.Allcock, F.W.Lampe and J.E.Mark, "Contemporary Polymer Chemistry", 3rd edn., Pearson, Prentice Hall, New Delhi, 2005.

Unit V: Polymer processing (9 hours)

Polymer processing – plastics (thermo and thermosetting), elastomers, fibres, compounding, plasticizers, colorants, flame retardants.

Compression and injection mouldings – film extrusion and calendaring – die casting and rotational casting – thermoforming – reinforcing.

Reference books :

1. J.A.Brydson, "Plastics Materials", 7th edn., Butterworth – Heinemann Publishers, New Delhi, 1999.
2. R.J.Crawford, "Plastics Engineering"3rd edn., Butterworth – Heinemann Publishers, Singapore, 1999.

Semester - IV - Part – III - Core Subject XI - Organic Chemistry IV

Hours per week: 5 **Credits: 4**

Subject Code: P19CHC41

Objectives:

- To get mastery over retrosynthesis.
- To study the structural elucidation of alkaloids, terpenoids and steroids.
- To learn ORD, CD and chromatographic techniques.
- To gain the basic knowledge in green chemistry.

Unit- I: Synthetic methods II **(15 hours)**

Functional group interconversions-diastereoselectivity-enanatioselectivity-stereoselectivity-regioselectivity- retrosynthetic analysis-carbon skeleton-functional group located on the skeleton-disconnection approach-basic principles-one group disconnection-two group disconnection-C-X disconnections-1,2-, 1,4-, 1,5- difunctionalized compounds-A schematic analysis of the total synthesis of the following compounds-2,4-dimethyl-2-hydroxypentanoic acid, trans-9-methyl-1-decalone and isonootkatone.

Reference Books

1. R.E.Ireland, Organic synthesis, Prentice – Hall of India Pvt. Ltd., 1975.
2. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part B, V Edn., Springer, New York, 2007.
3. W.Carruthers and Iain Coldhain, Modern Methods in Organic Synthesis, 4th Edn., Cambridge University Press, U.K., 2008.
4. I.L.Finar, Organic chemistry, Vol.II, English Language Book Society,1977.
5. Stuart Warren, Organic Synthesis, The disconnection approach, John Wiley Student edition, Singapore, 2000.

Unit-II: Chiroptical and analytical techniques **(15 hours)**

ORD and CD – principle - Cotton effect - Types of ORD curves - axial α-haloketone rule - Octant rule - Applications to determine the configuration and conformation of simple monocyclic and bicyclic ketones-Comparison of ORD and CD.

Chromatographic techniques: Principle and applications in organic chemistry – Column, TLC, Paper, GLC, HPLC, exclusion and ion exchange Chromatography.

Reference books:

1. I.L.Finar, Vol.II, 5th Edn., Pearson Education Ltd., New Delhi, 2011.
2. B.M.Silverstein, G.C.Bassler and T.C.Morrill, Spectrometric Identification of Organic Compounds Wiley, 5th Edn., McGraw Hill, New York, 1994.
3. E.L.Eliel, Stereochemistry of carbon compounds. McGraw Hill, 1989

4. Nasipuri, Stereochemistry of Organic Compounds, Wiley Eastern Ltd., New Delhi, 1991.
5. P.Crabbe, ORD and CD in chemistry and Biochemistry, Academic Press, 1972.
6. A.Braithwaite and F.J.Smith, Chromatographic Methods, Chapman and Hall, 4th Edn., 1985.

Unit- III: Terpenoids and steroids (15 hours)

Terpenoids : Classification – Structural elucidation of α-pinene, zingiberene, cadinene and squalene - Biosynthesis of terpenoids.

Steroids: Classification - conformational aspects of A/B cis and A/B trans steroids – Synthesis, structure (position of the hydroxyl group and double bond and nature of the side chain (Barbier-Wieland degradative study) and stereochemistry of cholesterol - male sex hormones – testosterone – female sex hormones - oestrone and progesterone - A basic idea about adrenocortical hormones - Cortisone (synthesis not included).

Reference books:

1. I.L.Finar, Vol.II, 5th Edn., Pearson Education Ltd., New Delhi, 2011.
2. Paul de Mayo, Chemistry of Terpenoids, Vol.I & II, Academic Press.
3. L.Fieser and Mary Fieser, Steroids, Reinhold, 1953.
4. W.Klyne, The Chemistry of Steroids, Methuen and Co., New york, 1965.

Unit IV: Alkaloids and Proteins (15 hours)

Alkaloids: Classification - general properties – general methods of elucidating the structure of the alkaloids - Structure, synthesis and stereochemistry of the following alkaloids - Quinine – Morphine - Lysergic acid – Biosynthesis of alkaloids.

Proteins and Nucleic acids: Peptides - End group analysis (N-terminal analysis-Edman method – Sanger method or DNP method-C-terminal analysis) - structural elucidation and synthesis of peptides - structural elucidation of Glutathione and Oxytocin- an elementary treatment on enzymes, coenzymes and nucleic acids – Genetic code - DNA and determine the base sequence of DNA.

Reference Books

1. I.L.Finar, Vol.II, 5th Edn., Pearson Education Ltd., New Delhi, 2011.
2. O.P.Agarwal , Chemistry of Organic Natural Products, Vol.I, Goel Publishing House, Meerut, 2008.
3. O.P.Agarwal, Chemistry of Organic Natural Products, Vol.II Goel Publishing House, Meerut, 2008
4. K.W. Benty, Alkaloids, Vol I &II Interscience 1957.
5. Pelletier, Chemistry of Alkaloids, Van Nostrand Reinhold publisher, 1st edition, January 1970.

Unit- V: Green chemistry (15 hours)

Introduction to Green chemistry- Definition- Need for Green chemistry- Goals of green chemistry-Principles of green chemistry – Planning a green synthesis in the laboratory(choice of starting materials-choice of reagents-choice of catalysts-choice of solvent-mode of supplying energy to a reaction) - general interest for solvent free processes – solvent free techniques – green solvents - Microwave synthesis - Introduction and characteristics of microwave heating –

interaction of microwave radiation with material- difference between conventional heating and microwave heating - applications and advantages of microwave heating over conventional heating (Microwave assisted reactions in water-Microwave assisted reactions in organic solvents-Microwave assisted solvent free reactions).

Reference books:

1. K.R.Desai, Green Chemistry (microwave synthesis) Himalaya Publishing House.Mumbai, 2005.
2. A.K.Ahluwalia, Green Chemistry, Narosa Publishing House, New Delhi, 2013.
3. R.Sanghi and M.M.Srivastava, Greeen Chemistry, Narosa Publishing House. New Delhi, 2003.
4. V.Kumar, An Introduction to Green chemistry, Vishal Publishing Co., Jalandhar, 2013.

Semester IV – Part III – Core Subject XII – Inorganic Chemistry IV

Hours per week: 5 **Credits: 4**

Subject Code: P19CHC42

Objectives:

- To review nuclear chemistry thoroughly
- To gain a detailed knowledge of lanthanides and actinides.
- To learn the fundamentals of solid state chemistry.
- To study the role of photochemistry in inorganic chemistry.

Unit I – Nuclear Chemistry (15 hours)

Transmutation reactions - Nuclear Q value – Capture cross section – Threshold energy and excitation function- types of nuclear reactions – spallation, fragmentation, transfer reactions – Buckshot hypothesis, fission and fusion.

Nuclear fission – mass distribution of fission products – liquid drop model for nuclear fission. Nuclear fusion - thermonuclear reaction in stars.

Nuclear reactor and its components: Nuclear materials – fissile and fertile isotopes - production of feed material for nuclear reactors – Nuclear waste disposal and radiation protection. Breeder reactor – Atomic power projects in India – Visit to Nuclear power plant.

Reference books

1. H.J. Arnikar, Essentials of Nuclear Chemistry, 4th edition, New Age Publishers New Delhi,
(2009).
2. S. Glasstone, Source book on Atomic energy, 3rd edition, East West Press, (1967).

Unit II – Chemistry of Lanthanides and Actinides (15 hours)

Lanthanides – occurrence, extraction from ores – separation procedure – ion exchange method – solvent extraction method. Properties of lanthanides – electronic configuration – common oxidation state – lanthanide contraction and its consequences – colour of lanthanide ions – spectral and magnetic properties of lanthanides.

Actinides – separation of actinide elements – separation of plutonium from fission products – electronic configuration – oxidation state – spectral and magnetic properties – comparison of lanthanides and actinides.

Reference books

1. J.E. Huheey, E.A. Keiter and R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity (4th edition): Addison-Wesley Publishing Company, New York, 1996.
2. F.A.Cotton and G.Wilkinson, Advanced Inorganic Chemistry (5th edition), John Wiley & Sons, New York, 1988.
3. J.D. Lee, Concise Inorganic Chemistry , 5th edition, Blackwell Science, 2000.
4. D.F.Shriver, P.W.Atkins and C.H.Langford, Inorganic Chemistry, 3rd edition, Oxford Univ. Press, 1999.
5. H.D. Mathur and O.P. Tandon, Chemistry of Rare Elements, IV Edn., S.Chand & Co.,1986.

Unit III – Solid State Chemistry – I (15 hours)

Principle and working of Rotating crystal method - X-ray diffraction - neutron diffraction – comparision of X-ray and neutron diffraction – electron diffraction – electron diffraction by gases – Applications of electron diffraction study.

Unit cell structure of zinc blende, wurtzite, fluorite, antifluorite, rutile and cesium chloride – spinels normal and inverse types and pervoskite structure.

Unit IV - Solid State Chemistry – II (15 hours)

Electronic structure of solids – Free electron and band theory – Band structure of metals, different types of semiconductors, insulators – Crystal defects – point, line and plane defects – colour centres – Formation of nonstoichiometric oxides and their properties – solid electrolytes and their applications –

Optical and electrical properties of semiconductors – photovoltaic effect – Hall effect – p-n and n-p-n junctions and their applications as rectifier and transistor – super conductivity – high temperature super conductors – Meissaner effect and levitation.

Reference books (Units III & IV)

1. L.V. Azaroff, Introduction to Solids, Tata-McGraw Hill (1977).
2. M.G. Arora Solid State Chemistry, Anmol Publishers New Delhi, (2001).
3. D. K. Chakrabarty Solid State Chemistry, New Age Publishers New Delhi, (2010).

Unit V – Inorganic Photochemistry (15 hours)

Electronic transition in metal complexes. Photophysical process of coordination compounds. Photochemical process of coordination compounds – photoisomerisation reaction – photosubstitution reaction – photoanation reaction – photoredox reaction. Photochemistry of cobalt(III) ammine complexes – photochemistry of chromium(III) ammine complexes – Adamson's rule. Photochemistry of ruthenium bipyridyl complexes. Photochemistry of organo metallic compounds – ligand photoreaction. Applications of metal complexes in solar energy conversion.

Reference books

1. Inorganic Chemistry, A Unified Approach, William W.Potterfield, Academic Press, An inprint of Elsevier, California (1993).
2. A.W. Adamson and F.D. Fleischer, Concepts of Inorganic Photochemistry, John Wiley – Inter Science, New York, 1975.
3. Arunachalam Inorganic photochemistry.

Semester - IV - Part – III - Core Subject XIII - Physical Chemistry IV

Hours per week: 5 **Credits: 4**

Subject Code: P19CHC43

Objectives:

- To learn the physical chemistry background for various spectral techniques.
- To study precisely colloids and surface chemistry
- To get a detailed knowledge in photochemistry.
- To study the role of physical aspects of some biological process

Unit I: **Spin Resonance Spectroscopy** **(15 hours)**

Magnetic properties of nuclei- Resonance condition - NMR instrumentation- Relaxation processes- Bloch equations- chemical shift - spin-spin splitting, relaxation times, line shape and line width analysis. Experimental techniques in NMR- double resonance technique- ENDOR, Overhauser effect, FT-NMR spectroscopy.

EPR- Principle of EPR- total Hamiltonian- Hyperfine structure- EPR of hydrogen atom- splitting in isotropic systems involving more than one nucleus- EPR spectra of free radicals in solution- methyl radical, benzene radical anion, *p*-benzosemiquinone radical anion, *p*-nitrobenzoate dianion and naphthalene anion.

Unit II: **NQR and Photoelectron Spectroscopy.** **(15 hours)**

Nuclear Quadrupole Resonance (NQR) spectroscopy - Principle of NQR- Transitions for axially and non-axially symmetric systems-Applications of NQR- Halogen, minerals and nitrogen - group frequencies –hydrogen bonding.

Photoelectron Spectroscopy- theory – XPS – UV-PES – instrumentation-evaluation of ionization potential – Chemical identification of element – Koopmans's theorem – Chemical shift – UPS – XPES of N_2, O_2 and HCl – evaluation of vibrational constants from UPS – spin – orbital coupling – Auger spectroscopy – principle and its application

Reference books:

1. G. Aruldhas, "Molecular Structure and Spectroscopy", Prentice-Hall of India Pvt., Ltd., New Delhi (2001).
2. G.R. Chatwal, S.K. Anand, Spectroscopy (Atomic and Molecular), Himalaya Publishing House, Mumbai, (2009).
3. P.Atkins, J. De Paula, Atkins' Physical Chemistry, Oxford University Press, New York, (2006).
4. G.K. Vemulapalli, Physical Chemistry, PHI Learning Pvt., Ltd., New Delhi (2009).
5. R.S.Drago, Physical Methods in Chemistry, W.B. Saunders Co., London (1977).
6. E.B.Becker, High Resolution NMR, 2nd edn,"Academic Press, (1990).
7. E.A.V. Ebsworth, D.W.H. Rankin, S.Cradock, "Structural Methods in Inorganic Chemistry", English Language Book Society / Black well Scientific Publications, (1987).

Unit III: **Colloids and Surface Chemistry** **(15 hours)**

Colloids: Different colloidal systems- characteristics of true solutions, colloidal solutions and suspensions- General properties of colloidal systems-coagulation, flocculation or precipitation of colloidal solution- Protective colloids- Gold number- Hardy-Schulze rule- Hofmeister series-

Electrokinetic phenomena including electro-osmosis and electrophoresis- Emulsions- Gels - Importance and applications of colloids.

Surface Chemistry: Introduction- Adsorption of gases on solids- physisorption and chemisorption- adsorption isotherms- Freundlich- Langmuir- BET – Temkin adsorption isotherms- surface area determination - Adsorption on liquid surface - surface tension- Gibbs adsorption isotherm.

Reference books:

1. D.J.Shaw, Introduction to Colloid and Surface Chemistry, Butterworth & Co. (Publishers) Limited (1968).
2. B.R. Puri, L.R. Sharma and M.S. Pathania, Principles of Physical Chemistry (Millennium Edn,) Vishal Publishing Co., (2003).
3. A.W. Adamson, Physical chemistry of surfaces, 5th Edn., John-wiley & Sons, New York (1990).
4. D. Attwood and A.T. Florence, Surfactant systems- Their chemistry, pharmacy and biology, Chappmann and Hall, New York (1983).

Unit IV: **Photochemistry** **(15 hours)**

Physical properties of the electronically excited molecules- excited state dipole moments, acidity constants (pKa^*-values) and redox potentials. Intermolecular deactivation of excited states- photosensitized reactions- Photophysical kinetics of intermolecular processes- Stern-Volmer equation and its applications - Excimer and excited state dimers.

Tools and techniques in photochemistry - light sources and their standardization chemical actinometry- conventional photolysis procedure. Measurements of emission characteristics- emission and excitation spectra- measurement of quantum efficiency determination of decay constants or radiative lifetimes. photochemical conversion and storage of solar energy.

Reference books:

1. K.K. Rohatgi-Mukherjee, Fundamentals of photochemistry, Wiley Eastern New Age International (P) Limited, Publishers, (1986).
2. J. Rajaram and J.C. Kuriakose, Kinetics and mechanisms of chemical transformations Applications of Femtochemistry, Macmillan India Ltd., (2008).
3. N.J. Turro, Modern Molecular photochemistry, Benjamin Cummings, (1965).
4. C. Kutal, Photochemical conversion and storage of solar energy, Journal of Chemical Education, **60**, (1983) p. 882-887.
5. J. Rajaram and J.C. Kuriakose, Thermodynamics for students of chemistry, Shoban Lal Nagin Chand & Co., (1986).
6. D.A. McQuarrie and J. D. Simon, Molecular Thermodynamics, Viva Books Pvt., Ltd., New Delhi (2004).

Unit V: **Biophysical Chemistry** **(15 hours)**

Basic concept of non-equi1ibrium thermodynamics – Onsager reciprocal relationship- Bioenergetics and metabolism-catabolism-anabolism-Energy relationship between catabolic and anabolic pathways- High energy metabolites - ATP and its role in bioenergetics – phosphoryl group transfers and ATP- Role of singlet oxygen in biology- Biophysical applications of Mossbauer effect- Mossbauer effect in hemoglobin- Molecular recognition- an introduction to supramolecular chemistry.

Recommended Books

1. M.M. Cox, D.L. Nelson, "Lehninger Principles of Biochemistry" 5th Edn., W.H. Freemman & Co., (2008).
2. Dickson, Dominic P.E. and Frank J. Berry, eds. Mössbauer Spectroscopy. Cambridge University
Press, New York: 1986.
3. U. Gosner and R.W. Grant, "Mossbauer Effect in Hemoglobin and Some Iron-Containing Biological Compounds." *Biophysical Journal* (5) (1965) p. 823-844.
4. Michael I Oshtrakh, "Mossbauer Spectroscopy in Biomedical Research", *Faraday Discussions,* **126** (2004) p.119-140.

Part III – Core Lab IV – LAB: Organic Chemistry Practical II

Hours per week: 4 **Credits: 4**

Subject Code: P19CHP41

Organic analysis and spectral interpretation

Objectives:

- To study the basics of separation and analysis of mixture of organic compounds.
- To interpret the UV, IR and NMR spectra of organic compounds.

Separation and analysis of the two component mixtures: Separation and analysis of the components, preparation of solid derivative and submission of physical constants for the components and its solid derivatives, identification of the components also from UV, IR and NMR spectral data.

Part III – Core Lab V – Inorganic Chemistry Practical II

Hours per week: 5 **Credits: 5**

Subject Code: P19CHP42

Quantitative analysis and Inorganic Preparation

Objectives:

- To practice quantitative estimation of more than one cation opting volumetric and gravimetric estimations.
- To practice the preparation of simple co-ordination compounds.
- To study the basics of photocolorimetric estimation of metals.

Quantitative estimation of a mixture containing two metal ions (volumetric and gravimetric estimations)
Estimation of Cu^{2+} and Ni^{2+}
Estimation of Cu^{2+} and Zn^{2+}
Estimation of Fe^{2+} and Cu^{2+}
Estimation of Fe^{2+} and Ni^{2+}
Estimation of Ca^{2+} and Mg^{2+}
Estimation of Ca^{2+} and Ba^{2+}
Analysis of ores and alloys (course work only)
Photocolorimetric estimation of metal ions (course work only)

Inorganic Complexes Preparation

Preparation of atleast 8 inorganic complexes.

For examination a mixture will be given from which one cation is to be estimated volumetrically and the other gravimetrically.

COURSE : II M.Sc. CHEMISTRY **SEMESTER : IV**	**Project & Viva-voce** **CORE LAB 5**	**Hours : 6** **Credit : 5**

Mark : 40 + 60 Marks Subject Code: P19CH4PV

Objectives:

The aim of project work (field/ lab work) is to inculcate students to learn adequate/ to enhance their knowledge/skills on research methodology/chemical industry process & R&D work in the subject and prepare them for pursuing research in *experimental or computational* areas of the subject or work in Industry. Students will be allotment by lot system. The project work / Field Work / Study carried out in Our College Chemistry Department or Field work in Chemistry or related Industry / National labs / University Labs /DAE Labs is to be undertaken under the guidance of a Teacher of the Department. The guiding teacher will make continuous internal assessment of the Project Work/ Field Study. No teacher shall be permitted to guide more than ***three*** students in a semester for Project Work/Field work / Study under his/her supervision. The project / Field work will be evaluated by the external examiner.

- Project will be done by the final year students in the fourth semester under the guidance of respective guides.
- For projects internal marks (max 50) will be awarded by the respective guide and external marks (max 50) will be awarded in the external examinations.
- Minimum number of Pages for M.Sc. Project thesis should be 35.

Course Name: Master of Science
Discipline: Chemistry
CHOICE BASED CREDIT SYSTEM
(For those who joined in June 2018 and after)
Course scheme:
Self Learning Courses:

Year	Semester	Subject	Credit	Ext =Tot	Subject Code
II	III	Applied Chemistry	5	100 = 100	P19CHSL31
II	III	CRITICAL ANALYSIS OF GATE/CSIR-NET QUESTIONS	5	100 = 100	P19CHSL32

Self Learning Course
APPLIED CHEMISTRY

Credit: 5 **Subject Code: P19CHSL31**
Total marks 100

Unit I FUELS

Classification of fuels – Calorific value- characteristics of a good fuel- Comparison between solid, liquid and gaseous fuels - Coal –chemical constitution and types – Petroleum - classification and composition- Petrol- Kerosene-Diesel- Comparative account of diesel and petrol – Cracking - Knocking - Octane rating - Diesel- index- Natural gas - Coal gas - Oil gas – Producer gas - Water gas- Biogas.

Reference:

1. P. C. Jain & M. Jain, Engineering Chemistry, Dhanpat Rai Publishing Company, 2000.
2. B. K. Sharma, Industrial Chemistry, Goel Publishing House, Meerut, India, 1994.

Unit II MATCH INDUSTRY

Advantages of Safety matches over Lucifer matches – Preparation, properties and uses of chemicals in matchstick head**:** $KClO_3$, KNO_3, Sulphur, Antimony sulphide, Borax, MnO_2, Wax, Glue and Potassium dichromate.

Body composition of colour and/or star matches: Colour matches: $KClO_3$, Barium nitrate, Strontium nitrate, Shellac, Lamp black, Paris green, Resin, Denatured sprit. Manufacturing process of matchsticks – Dipping process: Wax dipping and chemical dipping , drying - automation process.

Manufacture of conventional fireworks products: Flower pot, Ground chackra, Sparkles, Pencil, Crackers, Rockets and Atom bomb, Aerial Shots – Fuse making – Caps and ring caps – gun powder, serpent egg.

Reference:

1. P. L. Sony, "Text Book of Inorganic Chemistry" Mohan Katya Sultan Chand and Sons – New Delhi, 2013.
2. K. N. Ghosh, "The principles of fire works" 1987, Sivakasi.

UNIT-III VEGETABLE OIL INDUSTRY

Cleaning , Dehulling, Heat treatment of oil seeds, Rendering & Cooking types of rendering – Solvent extraction method of oil extraction – Various solvents used for solvent extraction - Modern extraction of gingelly oil from sesame seed.

Refining – effect of refining – types of refining – adsorption method- bleaching – chemical methods of bleaching – deodourisation.

Determination Acid Value (% FFA) – Iodine Value – Bellier Turbidity Temperature for gingelly and groundnut oils.

Reference:

1. C. Paquot, Standard methods for the analysis of Oils, Fats and Derivatives, 6th edition, Pergmon press, 1979.
2. E. A. Weiss, Oilseed Crops, Longman Group Limited, London, 1983.
3. F. D. Gunstone, An Introduction to the chemistry and Biochemistry of Fatty acids and their Glycerides, Chapman and Hall Ltd, 1967.
4. S.BP Board of Consultants and Engineers, Fatty Acids and Products, Small Business Publications, 1970.

UNIT-IV PAINTS AND PIGMENTS

Paints and pigments - formulation, composition and related properties. Oil paint, vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrode and electrolytic), metal spraying and anodizing.

Reference:

1. B. K. Sharma, Industrial Chemistry, Goel Publishing House, Meerut, India, 1994.
2. P. C. Jain & M. Jain, Engineering Chemistry, Dhanpat Rai Publishing Company, 2000.

UNIT V PLASTIC RECYCLING

Introduction to plastic wastes - Sources of plastic wastes - Generation of industrial plastic wastes- Plastics in solid wastes- Future of waste disposal - Primary recycling - Degradation of thermoplastics (Industrial practices) - Secondary Recycling - Approaches to secondary recycling - Chemical modification of mixed plastic waste - Secondary recycling by Co-extrusion & Injection molding - Use of waste plastics as Filler - Tertiary Recycling - Chemicals from waste - Pyrolysis - Chemical decomposition - Quaternary Recycling - Energy from plastic waste - Recycling of Various Plastics: HDPE, Acrylics, PET, PVC, Medical Plastics - Resin Identification Number (RIN) and its significance in recycling of plastics.

Reference:

1. Plastic Wastes in the Environment, Institute of European environmental Policy, 2011.
2. Good Practices Guide on Waste Plastic Recycling, by Local and Regional Authorities.

CRITICAL ANALYSIS OF GATE/CSIR-NET QUESTIONS

Credit: 5 **CODE: P19CHSL32**

Total Marks: 100

Course Outcomes:

Students, after successful completion of the course, will be able to

- Understand the fundamentals of chemistry concepts
- Apply and solve the chemistry problems
- Prepare for the competitive exam
- Pass the competitive exam successfully

Unit-I :

- **Equilibrium:** Laws of thermodynamics. Standard states. Thermochemistry. Thermodynamic functions and their relationships: Gibbs-Helmholtz and Maxwell relations, van't Hoff equation. Criteria of spontaneity and equilibrium. Absolute entropy. Partial molar quantities. Thermodynamics of mixing. Chemical potential. Fugacity, activity and activity coefficients. Chemical equilibria. Dependence of equilibrium constant on temperature and pressure. Non-ideal solutions. Ionic mobility and conductivity. Debye-Hückel limiting law. Debye-Hückel-Onsager equation. Standard electrode potentials and electrochemical cells. Potentiometric and conductometric titrations. Phase rule. Clausius-Clapeyron equation. Phase diagram of one component systems: CO_2, H_2O, S; two component systems: liquid-vapour, liquid-liquid and solid-liquid systems. Fractional distillation. Azeotropes and eutectics. Statistical thermodynamics: microcanonical and canonical ensembles, Boltzmann distribution, partition functions and thermodynamic properties.
- **Kinetics:** Transition state theory: Eyring equation, thermodynamic aspects. Potential energy surfaces and classical trajectories. Elementary, parallel, opposing and consecutive reactions. Steady state approximation. Mechanisms of complex reactions. Unimolecular reactions. Kinetics of polymerization and enzyme catalysis. Fast reaction kinetics: relaxation and flow methods. Kinetics of photochemical and photophysical processes.
- **Surfaces and Interfaces:** Physisorption and chemisorption. Langmuir, Freundlich and BET isotherms. Surface catalysis: Langmuir-Hinshelwood mechanism. Surface tension, viscosity. Self-assembly. Physical chemistry of colloids, micelles and macromolecules.

Unit-II :

- **Main Group Elements:** Hydrides, halides, oxides, oxoacids, nitrides, sulfides – shapes and reactivity. Structure and bonding of boranes, carboranes, silicones, silicates, boron nitride, borazines and phosphazenes. Allotropes of carbon. Chemistry of noble gases, pseudohalogens, and interhalogen compounds. Acid-base concepts.
- **Transition Elements:** Coordination chemistry – structure and isomerism, theories of bonding (VBT, CFT, and MOT). Energy level diagrams in various crystal fields, CFSE, applications of CFT, Jahn-Teller distortion. Electronic spectra of transition metal complexes: spectroscopic term symbols, selection rules, Orgel diagrams, charge-transfer spectra. Magnetic properties of transition metal complexes. Reaction mechanisms: kinetic and thermodynamic stability, substitution and redox reactions.

- **Lanthanides and Actinides:** Recovery. Periodic properties, spectra and magnetic properties.
- **Organometallics:** 18-Electron rule; metal-alkyl, metal-carbonyl, metal-olefin and metal-carbene complexes and metallocenes. Fluxionality in organometallic complexes. Types of organometallic reactions. Homogeneous catalysis - Hydrogenation, hydroformylation, acetic acid synthesis, metathesis and olefin oxidation. Heterogeneous catalysis - Fischer-Tropsch reaction, Ziegler-Natta polymerization.

Unit-III:

- **Reaction Mechanisms:** Basic mechanistic concepts – kinetic *versus* thermodynamic control, Hammond's postulate and Curtin-Hammett principle. Methods of determining reaction mechanisms through identification of products, intermediates and isotopic labeling. Nucleophilic and electrophilic substitution reactions (both aromatic and aliphatic). Addition reactions to carbon-carbon and carbon-heteroatom (N,O) multiple bonds. Elimination reactions. Reactive intermediates – carbocations, carbanions, carbenes, nitrenes, arynes and free radicals. Molecular rearrangements involving electron deficient atoms.
- **Organic Synthesis:** Synthesis, reactions, mechanisms and selectivity involving the following classes of compounds – alkenes, alkynes, arenes, alcohols, phenols, aldehydes, ketones, carboxylic acids, esters, nitriles, halides, nitro compounds, amines and amides. Uses of Mg, Li, Cu, B, Zn and Si based reagents in organic synthesis. Carbon-carbon bond formation through coupling reactions - Heck, Suzuki, Stille and Sonogoshira. Concepts of multistep synthesis - retrosynthetic analysis, strategic disconnections, synthons and synthetic equivalents. Umpolung reactivity – formyl and acyl anion equivalents. Selectivity in organic synthesis – chemo-, regio- and stereoselectivity. Protection and deprotection of functional groups. Concepts of asymmetric synthesis – resolution (including enzymatic), desymmetrization and use of chiral auxilliaries. Carbon-carbon bond forming reactions through enolates (including boron enolates), enamines and silylenol ethers. Michael addition reaction. Stereoselective addition to C=O groups (Cram and Felkin-Anh models).
- **Pericyclic Reactions and Photochemistry:** Electrocyclic, cycloaddition and sigmatropic reactions. Orbital correlations - FMO and PMO treatments. Photochemistry of alkenes, arenes and carbonyl compounds. Photooxidation and photoreduction. Di-π-methane rearrangement, Barton reaction.
- **Heterocyclic Compounds**: Structure, preparation, properties and reactions of furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline.

Unit-IV:

- **Structure:** Postulates of quantum mechanics. Time dependent and time independent Schrödinger equations. Born interpretation. Particle in a box. Harmonic oscillator. Rigid rotor. Hydrogen atom: atomic orbitals. Multi-electron atoms: orbital approximation. Variation and first order perturbation techniques. Chemical bonding: Valence bond theory and LCAO-MO theory. Hybrid orbitals. Applications of LCAO-MOT to H^{2+}, H_2 and other homonuclear diatomic molecules, heteronuclear diatomic molecules like HF, CO, NO, and to simple delocalized π– electron systems. Hückel approximation and its application to annular π – electron systems. Symmetry elements and operations. Point

groups and character tables. Origin of selection rules for rotational, vibrational, electronic and Raman spectroscopy of diatomic and polyatomic molecules. Einstein coefficients. Relationship of transition moment integral with molar extinction coefficient and oscillator strength. Basic principles of nuclear magnetic resonance: nuclear *g* factor, chemical shift, nuclear coupling.

- **Radioactivity:** Decay processes, half-life of radioactive elements, fission and fusion processes.
- **Bioinorganic Chemistry:** Ion (Na^+ and K^+) transport, oxygen binding, transport and utilization, electron transfer reactions, nitrogen fixation, metalloenzymes containing magnesium, molybdenum, iron, cobalt, copper and zinc.
- **Solids:** Crystal systems and lattices, Miller planes, crystal packing, crystal defects, Bragg's law, ionic crystals, structures of AX, AX_2, ABX_3 type compounds, spinels, band theory, metals and semiconductors.

Unit-V:

- **Stereochemistry**: Chirality of organic molecules with or without chiral centres and determination of their absolute configurations. Relative stereochemistry in compounds having more than one stereogenic centre. Homotopic, enantiotopic and diastereotopic atoms, groups and faces. Stereoselective and stereospecific synthesis. Conformational analysis of acyclic and cyclic compounds. Geometrical isomerism. Configurational and conformational effects, and neighbouring group participation on reactivity and selectivity/specificity.
- **Biomolecules**: Structure, properties and reactions of mono- and di-saccharides, physicochemical properties of amino acids, chemical synthesis of peptides, structural features of proteins, nucleic acids, steroids, terpenoids, carotenoids, and alkaloids.
- **Instrumental Methods of Analysis:** UV-visible spectrophotometry, NMR and ESR spectroscopy, mass spectrometry. Chromatography including GC and HPLC. Electroanalytical methods- polarography, cyclic voltammetry, ion-selective electrodes. Thermoanalytical methods.
- **Spectroscopy**: Applications of UV-visible, IR, NMR and Mass spectrometry in the structural determination of organic molecules.