SRI SARADA COLLEGE FOR WOMEN (AUTONOMOUS)

Reaccredited with 'B++' Grade by NAAC
Affiliated to Periyar University
Fairlands, Salem-636 016

PG & RESEARCH

DEPARTMENT OF CHEMISTRY

OUTCOME BASED SYLLABUS
M.Sc. CHEMISTRY

For the students admitted in 2022-23

(2022 – 2024 Batch)

M.Sc. Chemistry

PROGRAMME OUTCOMES (POs)

On completion of the programme, the students are expected to

PO No.	PO statement
PO1	possess deep and extensive knowledge on the key aspects and advanced concepts in chemistry.
PO2	plan, execute, record, interpret the observations and present the results of the chemical experiments.
PO3	have relevant knowledge, critical thinking, problem solving skills so as to enable them to face competitive exams and pursue research.
PO4	have gate way to varied avenues like research laboratories, industries and academic sectors.
PO5	design and perform interdisciplinary projects to meet the requirements related to the society.

SRI SARADA COLLEGE FOR WOMEN (AUTONOMOUS), SALEM -16
PG & RESEARCH DEPARTMENT OF CHEMISTRY
M.Sc. CHEMISTRY
PROGRAMME STRUCTURE UNDER CBCS
(For the students admitted in 2022-2023)
Total Credits: 92+Extra Credits (Maximum 16)
I SEMESTER

Course	Course Title	Code	Hrs./ Week	Credits
Core-I	Inorganic Chemistry-I	22PCHC1	5	5
Core-II	Organic Chemistry-I	22PCHC2	6	5
Core-III	Physical Chemistry-I	22PCHC3	5	5
Elective-I	Advanced Chemistry/ Water Chemistry	22PCHEC1/ 22PCHESC1	5	5
Core-IV	Inorganic Chemistry Practical	22PCHQC1	3	**
Core-V	Organic Chemistry Practical-I	22PCHQC2	3	**
Core-VI	Physical Chemistry Practical-I	22PCHQC3	3	**
	Total		**30**	**20**
Extra Skills	• *Value Education* • *Physical Fitness Practice* • *Life Skills Promotion* • *Productive Preparation for CSIR – UGC NET/SET/JRF – I (22PCHSC1) (Self Study – 1 Extra Credit)*			

II SEMESTER

Course	Course Title	Code	Hrs./ Week	Credits
Core-VII	Inorganic Chemistry-II	22PCHC4	6	5
Core-VIII	Organic Chemistry-II	22PCHC5	6	5
Elective–II	Chemical Kinetics and Thermodynamics/ Green Chemistry	22PCHEC2/ 22PCHESC2	6	5
Core-IV	Inorganic Chemistry Practical	22PCHQC1	3	3
Core-V	Organic Chemistry Practical-I	22PCHQC2	3	3
Core-VI	Physical Chemistry Practical-I	22PCHQC3	4	4
	Human Rights	22PHRSC	2	2
	Total		**30**	**27**
Extra Skills	• *Value Education – 1 Extra Credit* • *Physical Fitness Practice - 1 Extra Credit* • *Life Skills Promotion - 1 Extra Credit* • *Productive Preparation for CSIR – UGC NET/SET/JRF – II (22PCHSC2) (Self Study – 1 Extra Credit)* • *Society Connect Activity – 1 Extra Credit*			

• ***Extra credits are given for extra skills and courses qualified in*** **MOOC/ NPTEL**

III SEMESTER

Course	Course Title	Code	Hrs./ Week	Credits
Core-IX	Organic Chemistry-III	22PCHC6	5	4
Core-X	Physical Chemistry-II	22PCHC7	5	4
Core-XI	Coordination Chemistry	22PCHC8	5	4
Elective-III	Group Theory and Spectroscopy/ Nanochemistry	22PCHEC3/ 22PCHESC3	5	4
EDC	Therapeutical Chemistry	22PCHEDC	4	4
Core-XII	Organic Chemistry Practical-II	22PCHQC4	3	**
Core-XIII	Physical Chemistry Practical-II	22PCHQC5	3	**
	Total		**30**	**20**
Extra Skills	• *Value Education* • *Physical Fitness Practice* • *Life Skills Promotion* • *Productive Preparation for CSIR – UGC NET/SET/JRF – III (22PCHSC3) (Self Study – 1 Extra Credit)*			

- ***Preparation for the Project – 5 Hours per Week (Outside College Hours)***

IV SEMESTER

Course	Course Title	Code	Hrs./ Week	Credits
Core-XIV	Physical Methods in Chemistry	22PCHC9	6	5
Elective –IV	Introduction to Cheminformatics and Computer Aided Drug Design/ Solid State Chemistry	22PCHEC4/ 22PCHESC4	6	5
Elective –V	Organic Photochemistry and Spectroscopy/ Medicinal Chemistry	22PCHEC5/ 22PCHESC5	6	5
Core-XII	Organic Chemistry Practical-II	22PCHQC4	3	3
Core-XIII	Physical Chemistry Practical-II	22PCHQC5	3	3
Core-XV	Project	22PCHPC	6	4
	Total		**30**	**25**
Extra Skills	• *Value Education –1 Extra Credit* • *Physical Fitness Practice - 1 Extra Credit* • *Life Skills Promotion - 1 Extra Credit* • *Productive Preparation for CSIR – UGC NET/SET/JRF – IV(22PCHSC4) (Self Study – 1 Extra Credit)* • *Society Connect Activity – 1 Extra Credit*			

- ***Extra credits are given for extra skills and courses qualified in*** **MOOC/ NPTEL**

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : CORE-I: INORGANIC CHEMISTRY- I

COURSE CODE : 22PCHC1 HOURS/WEEK: 5 CREDITS: 5

SEMESTER : I

Course Objectives:

- *To study about nuclear chemistry and radiation chemistry*
- *To know the applications of radioactive isotopes*
- *To learn about structure and bonding of boron cage compounds, metal carbonyls and nitrosyls*
- *To understand the inorganic polymers such as Si, P and S.*
- *To acquire knowledge about electron transfer reactions*

Syllabus

UNIT-I **15 Hours**

Nuclear Chemistry-I

1.1. Nuclear structure-sub-atomic particles, nuclear properties - nuclear radii, nuclear spin and moments, nuclear forces-meson field theory, Salient feature of liquid drop model and shell model.

1.2. Artificial radioactivity, positron emission, orbital electron capture, nuclear isomerism and internal conversion.

1.3. Detection and determination of activity - Cloud chamber, Bubble chamber, GM, Scintillation and Cherenkov counters.

UNIT-II **15 Hours**

Nuclear Chemistry II

2.1. Natural radioactivity: α decay-tunnel effect, β-decay-types - β^+ and β^- - range of α and β radiation - Geiger-Nuttall rule, units of radioactivity.

2.2. Application of radioactive isotopes as tracers and chemical investigations, radiation protection and safety precautions.

2.3 Analytical applications - neutron activation analysis, isotope dilution analysis - industrial and medicinal application.

Radiation Chemistry

2.3. Radiation dosimetry, radiolysis of water and the hydrated electron.

UNIT – III **15 Hours**

Boron compounds and Clusters

3.1. Boron cage compounds- Diboranes- preparation, properties and bonding in higher boranes – B_4H_{10}, B_5H_9, B_6H_{10}, B_5H_{11}, $B_{10}H_{14}$ and $[B_{12}H_{12}]^{2-}$ and structures, calculation of framework electron, styx numbers, wade's rule,

3.2 Carboranes - types such as closo, nido -preparation, properties and structures. Metallocarborane - a general study.

3.3 Polyacids – Structural aspects of isopoly acids of V, Cr, Mo and W and heteropoly acids of Mo and W.

UNIT – IV **15 Hours**

Inorganic Polymers

4.1. Silicates -types of silicates (structural study only), Zeolites, Silicon based polymer: Silicone rubber, silicone greases, silicone resins and high thermal silicones.

4.2. Phosphorous based polymers: –Phosphonitrilic compounds (Phosphazenes)-linear, trimer and tetramer structures, preparation of $(PNCl_2)_3$, $(PNBr_2)_3$ and $(PNF_2)_3$, structure of $(PNCl_2)_3$, Craig and Peddock model, Dewar model.

4.3. Sulphur based polymers: Polymeric sulphur-S_4N_4-Polymeric sulphur nitride $(SN)_n$

UNIT – V

Electron transfer Reactions and Organometallic compounds **15 Hours**

5.1 Electron transfer reactions – Inner sphere (ISET) and outer sphere (OSET) electron transfer processes. Role of bridging ligand with ISET reaction – tunneling transfer – multiple bridging in the activated complex in the ISET process. Complimentary and non complimentary ET reactions. Cross reactions and Marcus Hush theory.

5.2 Metal carbonyls: structure and bonding of simple and polynuclear carbonyls, Infrared spectra of metal-carbon bond, Isolobal concepts.

5.3 Nitrosyls-bridging and terminal nitrosyls, bent and linear nitrosyls.

BOOKS FOR STUDY:

1. Arnicker, H. J., *Essentials of Nuclear Chemistry*, 4th Ed., New Age International (P) Ltd., 2003.
2. Shriver & Atkins, *Inorganic chemistry*, 4th Ed., Oxford University Press, 2006.
3. Puri, B. R., Sharma, L. R., Kalia, K. C., *Principles of Inorganic Chemistry*, 33rd Ed., Vishal Publishing Co., 2016.
4. Catherine E Housecroft., *The Heavier d-Block Metals: Aspects of Inorganic and Coordination Chemistry*, 1st Ed., Oxford university press, 1999.

BOOKS FOR REFERENCE:

1. Greenwood, N. N., & Earnshaw, A., *Chemistry of the Elements*. 2nd Ed., Butterworth Heinemann Linacre House, Jordan Hill, Oxford, 1997.
2. Keith, F., Purcell & John Kotz, C., *Inorganic Chemistry*, WB Saunders Co., USA, 1985.

3. James E Huheey., Ellen A Keiter., Richard L Keiter & Okhil K Mehdi., *Inorganic Chemistry-Principles of Structure and Reactivity*, 4th Ed.,2006.

WEB SOURCES:

1. https://preparatorychemistry.com/Bishop_Book_atoms_16.pdf
2. https://cd1.edb.hkedcity.net/cd/science/chemistry/s67chem/pdf/tOL_5_Silicates.pdf

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	illustrate the artificial radioactivity based on the concepts of nuclear chemistry	K2
CO2	utilize the radioactivity for various application	K3
CO3	determine the structure of boranes, carboranes, carbonyls and nitrosyls	K5
CO4	analyse the inorganic polymers and their structural models	K4
CO5	predict the electron transfer reactions of metal complexes	K6

K2-Understand; K3-Apply; K4-Analyse; K5-Evaluate; K6-Create

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	L	S	S	S
CO2	S	L	S	S	S
CO3	S	M	S	S	M
CO4	S	M	S	S	S
CO5	S	M	S	S	S

S-Strong; M-Medium; L- Low

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PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : CORE-II: ORGANIC CHEMISTRY- I

COURSE CODE : 22PCHC2 HOURS/WEEK: 6 CREDITS: 5

SEMESTER : I

Course Objectives:

- *To get exposed to the stereochemistry of organic compounds based on the spatial orientation of constituent atoms or groups.*
- *To acquire knowledge about conformational analysis of cyclic compounds, dynamic stereochemistry and reactivity.*
- *To understand and apply the effect of structure on reactivity and to know the various methods of determining reaction mechanisms.*
- *To understand the mechanisms of aliphatic and aromatic compounds towards nucleophilic substitution.*
- *To appreciate the reactivity of aliphatic and aromatic compounds towards nucleophilic substitution and the factors affecting them.*

Syllabus

UNIT – I **18 Hours**

Stereochemistry- I

1.1 Stereoisomerism -optical isomerism-definitions –conventions used in chemistry- Wedge, Newmann, Sawhorse and Fischer notations and interconversions- concept of chirality- principles of symmetry- classification of chiral molecules as asymmetric and dissymmetric

1.2 Molecules with axial chirality, planar chirality and helical structures- a brief study of dissymmetry of allenes, biphenyls, spiranes, alkylidene cycloalkanes, ansa compounds, cyclophanes, transcyclooctene and hexahelicene. Specification of R & S configuration to simple compounds, allenes, spirans and biphenyls-enantiomeric excess and optical purity. Biological importance of chirality- receptors- chiral drugs-Penicillamine, Thalidomide, Salbutamol, Ibuprofen.

1.3 Compounds with more than one chiral centre- calculation of number of stereoisomers- Erythro and threo nomenclature-stereospecific and stereoselective synthesis with suitable examples- asymmetric synthesis, Cram's rule, Felkin-Ahn model.

1.4 Topicity and prochirality- homotopic, enantiotopic, diastereotopic ligands and faces- concept of pro-R, pro-S, Re and Si faces- prochiral carbons.

UNIT – II **18 Hours**

Stereochemistry- II

2.1 Conformational analysis of cyclohexane, Stabilisation of flexible conformers. conformational analysis of mono and disubstituted cyclohexanes.

2.2 Conformational analysis of a few atypical disubstituted cyclohexanes, cyclopentane and cyclohexanone, 2-alkyl and 3-alkylketone effect- 2-halocyclohexanone. Conformational analysis of cyclooctane and trans annular interactions. Conformational analysis of cis and trans-decalin, 9- Methyldecalin.

2.3 Conformation and reactivity - substituted cyclohexanols (acylation and oxidation)- cyclohexane carboxylic acid derivatives (hydrolysis of ester) -nucleophilic substitution and elimination reactions in cyclohexane ring systems.

UNIT-III **18 Hours**

Structure and Reactivity

3.1 Resonance and field effects- Hammett equation and Linear Free Energy Relationship- substituent and reaction constants- Physical significance of σ and ρ- application to characterization of reaction mechanisms- simple problems-Taft equation.

3.2 Thermodynamic and kinetic requirements for reactions-Hammond's postulate - Microscopic reversibility- Curtin Hammett principle –transition states and intermediates.

3.3 Kinetic and non-kinetic methods of determining reaction mechanisms- Primary and secondary kinetic isotopic effects- identification of products and study of intermediates- isotopic labeling and cross over experiments.

UNIT-IV **18 Hours**

Aliphatic Nucleophilic Substitution

4.1 Types of aliphatic nucleophilic substitution -S_N1, S_N2 & S_Ni mechanisms - evidences- kinetic and stereochemical characteristics- comparison of the SN2 and SN1 reactions.

4.2 Neighbouring group participation, various cases of neighbouring group participation- heteroatoms as neighbouring groups (S, O and X)- nonclassical carbocations- π bonds as neighbouring group- norbornenyl and phenyl systems- C — C σ bond as a neighbouring group - norbornyl systems. Nucleophilic substitution at allylic, vinylic and bridgehead carbon, nucleophilic acyl substitution.

4.3 Factors affecting aliphatic nucleophilic substitution reactions- Distinction between nucleophilicity and basicity. Effect of substrate structure, attacking nucleophile, leaving group

and reaction medium on the rate- ambident nucleophiles- "O" Vs "C" alkylation- alkylation of active methylene compounds- regioselectivity.

4.4 Biological nucleophilic substitution-S-Adenosylmethionine.

UNIT-V **18 Hours**

Aromatic nucleophilic substitution

5.1 Study of the following reactions – Von Braun reaction, hydrolysis of ester- mechanism of BAC2, AAC2 and AAL1 only-Claisen and Dieckmann condensation-Finkelstein reaction and Wurtz coupling.

5.2 Aromatic nucleophilic substitution-Aryl halides- S_NAr- nucleophilic substitution involving diazonium ions- S_N1- benzyne mechanism, cine substitution-methods of generation of benzyne intermediate, trapping of aryne intermediates- reactivity – effect of substrate structure.

5.3 Zeigler alkylation, Chichibabin reaction, Schiemann reaction and Von-Richter rearrangement.

BOOKS FOR STUDY

1. P.S. Kalsi, *Stereochemistry, Conformation and Mechanism*, Sixth Ed., Wiley Eastern Limited, 2005.
2. D. Nasipuri, *Stereochemistry of Organic Compounds*, Second Ed., New York International Publishers, 1994.
3. R.T. Morrison and Boyd, *Organic chemistry*, Sixth Ed., Prentice Hall, 1992.

BOOKS FOR REFERENCE

1. Michael B. Smith & Jerry March, *March's Advanced Organic Chemistry- Reactions, Mechanisms and Structure*, Sixth Ed., John Wiley and Sons 2007.
2. Francis A. Carey, *Organic Chemistry*, Third Ed., The McGraw Hill Companies, Inc. 1996.
3. I.L. Finar, *Organic Chemistry*, Volume II, Fifth Ed., Pearson Education Asia Private Ltd. 2000.

Web Sources:

1. https://www.masterorganicchemistry.com/2012/04/17/homotopic-enantiotopic-diastereotopic/
2. https://nptel.ac.in/content/storage2/nptel_data3/html/mhrd/ict/text/104105086/lec10.pdf
3. http://content.inflibnet.ac.in/data-server/eacharya-
4. https://www.coursehero.com/file/44100228/1515564176CHE-P1-M17-etextpdf/
5. https://epgp.inflibnet.ac.in/view_f.php?category=

Course Outcomes

On successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	explain the different projection formulae, stereochemistry of reactions, identify the configuration, prochirality, chirality and the topical relationship in organic molecules	K4
CO2	examine the stability of various conformers of cyclic systems and correlate them to reactivity	K4
CO3	relate the effect of structure on reactivity, explain the kinetic and thermodynamic requirements of reactions and different methods of determining reaction mechanisms	K3
CO4	explain the different types of mechanism and factors affecting aliphatic and aromatic nucleophilic substitution reactions	K5
CO5	predict the major and minor products of aliphatic and aromatic nucleophilic substitution reactions with appropriate stereochemistry and regiochemistry and give synthetic routes for synthesis	K6

K3-Apply; K4-Analyse; K5-Evaluate; K6-Create

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	S	S	S	M
CO2	S	S	S	S	S
CO3	S	M	M	S	S
CO4	S	S	S	S	S
CO5	S	S	S	S	S

S-Strong; M-Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : CORE-III: PHYSICAL CHEMISTRY-I

COURSE CODE : 22PCHC3 HOURS/WEEK: 5 CREDITS: 5

SEMESTER : I

Course Objectives:

- *To understand the concepts and application of thermodynamics*
- *To understand and explore the reaction kinetics of complex and fast reactions*
- *To learn the basic concepts, principles and applications of quantum mechanics*
- *To understand the quantum mechanical treatment of simple systems.*
- *To learn the quantum mechanical treatment of multi electron systems.*

Syllabus

UNIT-I **15 Hours**

Classical Thermodynamics

1.1. Concepts of Partial Molar Properties-Partial Molar Free Energy and Partial Molar Volume - Gibbs-Duhem equation, Van't Hoff isotherm.

1.2. Chemical potential- Determination of chemical potential (direct method and method of intercepts)-Variation of chemical potential with temperature and pressure.

1.3. Fugacity–Determination of fugacity of gases by graphical method- Determination of fugacity from equation of state - Variation of fugacity with temperature and pressure - Lewis Randal rule-Duhem - Margules equation. Determination of activity and activity coefficient of non-electrolyte (e.m.f method)-Excess functions.

UNIT-II

Chemical Kinetics **15 Hours**

2.1 Kinetics of complex reactions – reversible reactions, consecutive reactions – Parallel reactions and Chain reactions.

2.2. Rice–Herzfeld mechanism for hydrogen-bromine, gas phase pyrolysis of methane and formation of phosgene reactions- explosion limits.

2.3. Study of fast reactions: Relaxation methods-temperature and pressure jump methods - Stopped flow technique, flash photolysis, nuclear magnetic resonance method and Crossed molecular beam method.

UNIT –III **15 Hours**

Quantum Chemistry-I

3.1 Black body radiation- Planck's quantum theory(derivation not needed) photoelectric effect- Wave particle duality.

3.2 Uncertainty principle - Compton effect - Operators-addition, subtraction, multiplication, linear, commutation, vector, Laplacian, Hermitian, Hamiltonian and momentum operators.

3.3 Eigen functions and Eigen values - Postulates of quantum mechanics. Derivation of Schrodinger's time-independent equation- Application of Schrödinger equation to a particle in one, two and three dimensional boxes – condition for normalisation and orthogonality.

UNIT-IV **15 Hours**

Quantum Chemistry - II

4.1 Application of Schrödinger equation to Simple harmonic oscillator and Rigid rotator.

4.2 Application of Schrödinger equation in arriving solution for wave function of the Hydrogen atom- Slater type orbitals-Slater rules.

4.3 Approximation methods-Perturbation method (upto second order in energy) and variation methods and their application to helium atom.

UNIT-V **15 Hours**

Quantum Chemistry-III

5.1. Born-Oppenheimer approximation-LCAO-MO approximation for hydrogen molecule ion -Valence bond theory of hydrogen molecule.

5.2. Concept of hybridization - sp, sp^2 and sp^3 hybridisation. LS-coupling and jj-coupling-term symbols (only ground state term symbol for simple atoms and 3d transition series).

5.3. Huckel molecular orbital (HMO) theory for conjugated π-system-applications to simple systems-(ethylene, butadiene and benzene)-self consistent field approximation-Hartree's and Hartree-Fock self consistent field theory.

BOOKS FOR STUDY:

1. Glasstone. S., *Thermodynamics for Chemists,* 11th Ed., Affiliated East West Press, 2008.

2. Puri, B.R., Sharma, L.R., Pathania, M.S., *Principles of Physical Chemistry*, 41st Ed., Vishal Publications, 2004.

3. Rajaram, J, Kuriacose J. C. *Thermodynamics for Students of Chemistry*, Lal Nagin Chand, New Delhi, 1986.

4. Prasad, R.K., *Quantum Chemistry*, 3rd Ed., Wiley Eastern Ltd., 1985.

BOOKS FOR REFERENCE:

1. Levine, I.N., *Quantum Chemistry,* 5th Ed., Pearson Prentice hall, 2000.

2. Chandra, A.K., *Introduction to Quantum Chemistry*, 4th Ed., Tata McGraw Hill, 1994.

WEB SOURCES:

1. http://www.iiserpune.ac.in/~p.hazra/FULL_Thermodynamics_lecture.pdf

2. http://ursula.chem.yale.edu/~batista/classes/vvv/v570.pdf

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	discuss the basic idea of classical thermodynamics, kinetics of complex reactions, fast reactions and quantum chemistry	K2
CO2	explain the concept of classical thermodynamics, kinetics of complex and fast reactions and quantum chemistry	K4
CO3	evaluate simple and multi electronic system quantum mechanically	K4
CO4	summarize the theories related to classical thermodynamics, kinetics of complex reactions, fast reactions and quantum chemistry	K4
CO5	solve the problem related to classical thermodynamics and quantum chemistry	K5

K2-Understand; K3-Apply; K4-Analyse; K5-Evaluate

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	S	S	S	S
CO2	S	S	S	S	S
CO3	S	L	S	S	S
CO4	S	M	S	S	S
CO5	S	L	S	S	S

S-Strong; M-Medium; L- Low

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : ELECTIVE – I: ADVANCED CHEMISTRY

COURSE CODE : 22PCHEC1 HOURS/WEEK: 5 CREDITS: 5

SEMESTER : I

Course Objectives:

- *To understand the principles, instrumentation and applications of the modern separation techniques GLC and HPLC.*
- *To impart knowledge about the principles, instrumentation and applications of Thermo analytical methods and Polarography.*
- *To learn the principles, instrumentation and applications of Coloumetry, and Amperometry.*
- *To know the principles, instrumentation and applications of AAS, AES and EDAX.*
- *To acquire knowledge about the advances in nanotechnology.*

Syllabus

UNIT-I 15 Hours

1.1. GLC-Principle, instrumentation, carrier gas, column preparations, types of detectors-Thermal conductivity, Flame ionization, Electron capture detectors.

1.2. HPLC-Scope, column efficiency, instrumentation, pumping systems, column packing, detectors.

1.3 Applications of GLC and HPLC.

UNIT –II 15 Hours

2.1 Thermogravimetry: Principle, factors affecting thermogram, instrumentation and applications of TGA, Differential techniques: Principles, factors affecting thermogram, instrumentation and applications of DTA, DSC and DTG.

2.2 Polarography – Basic Principle, instrumentation, factors affecting limiting current, residual current, migration current, diffusion current, half wave potential.

2.3 Applications of polarography-Determination of Cadmium in solution (wave height-concentration plot and method of standard addition), determination of lead and copper in steel.

UNIT – III 15 Hours

3.1 Coulometry: Principle, controlled potential coulometry and separation of nickel and cobalt, coulometric titration, instrumentation, Estimation of Sb(III).

3.2 Amperometry-Basic principle, instrumentation, Amperometric titration. Determination of lead with dichromate, sulphate with lead nitrate solution using amperometric method.

UNIT – IV 15 Hours

4.1 Atomic absorption spectroscopy-Basic principle, instrumentation, advantage over Flame photometry, detection limit, interferences – Applications.

4.2 Principle, theory, instrumentation and applications of AES.

4.3 Principle, theory, instrumentation and applications of EDAX.

UNIT- V **15 Hours**

Nanotechnology

5.1. Introduction, importance-various stages of nanotechnology, nanoparticles, Fullerenes.

5.2. Nano dendrimers - Nanopore channels, Fibres and scaffolds.

5.3. CVD diamond technology-FCVA technology and its applications, nano imaging techniques.

BOOKS FOR STUDY:

1. Arthur Israel Vogel, John Bassett., *Vogel's Text Book of Quantitative Inorganic Analysis*, 4th Ed., Longman Sc. & Tech. 1980.
2. Gurdeep Chatwal, Sham Anand, *Instrumental methods of Chemical Analysis*, 5th Ed., Himalaya Publishing House, 2007.

BOOKS FOR REFERENCE:

1. Douglas A. Skoog, Donald M. West, James Holler, F, Stanley R. Crouch., *Fundamentals of Analytical Chemistry*, 9th Ed., Belmont, CA : Brooks/Cole, Cengage Learning Publisher, 2014.
2. Mahinder Singh, *A Textbook of Analytical Chemistry*, 1st Ed., Dominant Publishers and Distributors, 2005.
3. Mick Wilson, *Nanotechnology-Basic Science and Emerging Technologies*, 1st Ed., Overseas Press Private Ltd. 2008.
4. Ewing G.W, *Instrumental Methods of Chemical Analysis*, McGraw Hill Publishers, 1975.

WEB SOURCES:

1. https://www.researchgate.net/publication/301700056_Gas_Liquid_Chromatography
2. https://laboratoryinfo.com › Biochemistry
3. https://www.researchgate.net/publication/235987484_High_performance_liquid_chromatography_A_short_review
4. scholar.cu.edu.eg › files › polarography
5. https://www.researchgate.net/publication/308371884_Atomic_Absorption_Spectroscopy_AAShttps://www.researchgate.net/publication/329380844_Amperometry
6. http://www.as.utexas.edu/astronomy/education/fall08/scalo/secure/309l_oct09_protein.pdf
7. https://www.britannica.com/science/fullerene

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	explain the concepts of GLC, HPLC, TGA, DTA, DTG, DSC, Polarography, Coloumetry, Amperometry, AAS, AES and EDAX	K2
CO2	outline the instrumentation of GLC, HPLC, TGA, DTA, DTG, DSC, Polarography, Coloumetry, Amperometry, AAS, AES and EDAX	K2
CO3	apply GLC, HPLC, TGA, DTA, DTG, DSC, Polarography, Coloumetry, Amperometry, AAS, AES and EDAX for analysis	K3
CO4	analyse the factors affecting GLC, HPLC, TGA, DTA, DTG, DSC, Polarography, Coloumetry, Amperometry, AAS, AES and EDAX	K4
CO5	categorize and characterize nanomaterials	K4

K2-Understand; K3-Apply; K4-Analyse

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	S	M	S	S
CO2	S	S	M	S	S
CO3	S	S	M	S	S
CO4	S	S	M	S	S
CO5	S	M	M	S	S

S-Strong; M-Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : ELECTIVE-I: WATER CHEMISTRY

COURSE CODE : 22PCHESC1 HOURS/WEEK: 5CREDIT: 5

SEMESTER : I

Course Objectives:

- *To understand the water quality parameters and disinfectants methods.*
- *To learn about the waste water treatment methods.*

SYLLABUS

UNIT – I **15 Hours**

Introduction

Sources of water, unique properties of water- water characteristics - water pollution-waste water generation.

Classification of water pollutants, constituents and characteristics of waste water.

Measurement techniques -sampling, colour & odour, dissolved oxygen, BOD, COD, TOC, N&P, suspended solids and bacteriological measurements.

UNIT – II **15 Hours**

Potable water

Potable water standards-WHO and other standards-bacteriological standards.

Disinfectants methods-oxidation method-bleaching powder, chlorine, ozone and UV.

Desalination - reverse osmosis and dialysis, nanofilteration.

UNIT – III **15 Hours**

Waste water treatment

Waste water treatment-pretreatment -screening, grit removal and pre- chlorination.

Primary treatment-settling and sedimentation.

Secondary treatment -trickling filter process, activated sludge process, Aeration.

UNIT – IV **15 Hours**

Industrial waste water treatment

Industrial waste water treatment - activated sludge treatment plants – mass balances, with and without recycle plants-single tank, contact stabilisation, biosorption plants.

Biofilters - Hydraulic film diffusion, two component diffusion -types of plants - trickling filters.

4.3 Submerged filters and rotating disc, removal of particulate organic matter.

UNIT – V **15 Hours**

Treatment plants

Treatment plants for nitrification-mass balances- nitrifying plants and types of plants.

Treatment plant for denitrification - mass balances-denitrifying plants and types of plants, redox zones in the biomass.

Anaerobic waste water treatment -Plant types, pretreatment, plant with suspended sludge and filter process.

BOOKS FOR STUDY:

1. De, A. K., *Environmental Chemistry*, Wiley Eastern Co., 2016.
2. Banerji, S. K., *Environmental Chemistry*, 2nd Ed., Prentice Hall of India, New Delhi, 2007.

BOOKS FOR REFERENCE:

1. Saxena, M. M., *Environmental Analysis of Water, Soil and Air*, Agro Botanica, 2nd Ed., Bikaner, 1990.
2. Ghosh, B., Bajaj, J. C., Hasan, R., & Singh. D., *Soil and Water Testing Methods, A Laboratory Manual*, IARI, New Delhi, 1983.

WEB SOURCES:

1. https://www.organicawater.com/primary-secondary-tertiary-wastewater-treatment-work/
2. https://www.ias.ac.in/article/fulltext/reso/005/11/0056-0068

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	assess the water quality parameters	K5
CO2	compare potable water standards and utilize different methods to improve water quality	K4
CO3	categorize waste water treatment methods	K4
CO4	plan industrial waste water treatment methods	K3
CO5	identify treatment plants	K4

K3-Apply; K4-Analyze; K5-Evaluate

Mapping of COs with POs

COs	**POs**				
	PO1	PO2	PO3	PO4	PO5
CO1	S	S	S	S	S
CO2	S	S	S	S	S
CO3	S	S	S	S	S
CO4	S	S	S	S	S
CO5	S	M	S	S	S

S-Strong; M-Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY
COURSE TITLE : CORE-VII: INORGANIC CHEMISTRY-II
COURSE CODE : 22PCHC4 HOURS/WEEK: 6 CREDITS: 5
SEMESTER : II

Course objectives

- *To improve sound knowledge in contemporary inorganic chemistry.*
- *To gain knowledge on the concept of coordination compounds.*
- *To understand the HSAB concepts.*
- *To learn about the action of biologically important complexes.*

SYLLABUS

UNIT I **18 hours**

Structural Aspects

1.1. Geometry and coordination numbers (two - six) and high (seven and above) coordination numbers, generalizations about coordination numbers and factors favouring high coordination numbers, macrocyclic ligands - types – porphyrins, corrins and Schiff's bases.

1.2. Kinetic reactivity and thermodynamic stability with examples - stepwise and overall stability constants, factors affecting the stability of a complex ion, chelate effect and its applications, determination of stability constant by polarographic, spectrophotometric and potentiometric methods.

1.3. Stereochemical aspects-stereoisomerism in inorganic complexes and ligand conformation.

UNIT-II **18 hours**

Metal-Ligand Bonding

2.1. Crystal field theory-crystal field effects in octahedral, tetrahedral and square planar symmetries, d-d transition, factors affecting the magnitude of Δ_o, CFSE-weak and strong field effects, colour and magnetic properties of transition metal complexes, applications of CFT, Irwing-Williams series, spectrochemical series, Jahn-Teller distortion- Jahn -Teller effect, evidences for metal-ligand overlap-esr, nmr, nephelauxetic effect, limitations of CFT.

2.2. MO theory and energy level diagram, concept of weak and strong field, sigma and pi-bonding in octahedral, tetrahedral complexes, sigma bonding in square planar complex-experimental evidence for pi bonding - IR spectra.

2.3. Nucleophilic substitution reaction - trans effect, trans influence, trans directing series, theories of trans effect, applications of trans effect.

UNIT-III **18 hours**

Solid State Chemistry

3.1. Structure of NiAs, CdI_2, pervoskite, rutile, fluorite and antifluorite, spinels and inverse spinels, defects in solids-point defects-line defects and surface defects, non- stoichoimetric compounds.

3.2. Electrical properties of solids: band theory, explanation of insulators, conductors, semiconductors and super conductors.

3.3. Diffusion types and mechanism: vacancy, interstitial, interstitialcy and ring diffusions, solid solution and order-disorder transformation and super structures.

UNIT-IV **18 hours**

4.1**. Hard and soft acids and bases:** HSAB - Pearson's principle, classification, symbiosis, theoretical basis of hardness and softness, electronegativity and hardness and softness, applications of HSAB.

4.2. Solid state electrolytes, reaction in solid state and phase transitions, magnetic properties - dia, para, ferro, anti-ferro and ferrimagnetism, hysteresis, ferrites, garnets, optical properties-solid state lasers and inorganic phosphors.

4.3. **Supramolecular chemistry**: Introduction-self assembly into mono and multilayer structure-applications of crown ethers, crypts and fullerenes.

UNIT-V **18 hours**

Bio- Inorganic Chemistry

5.1. Metal ions in biological systems-essential and trace metals.

5.2. Biologically important complexes - structure and functions of haemoglobin- cooperative effect, Bohr effect, trigger mechanism, myoglobin, hemerythrin and hemocyanin, electron transfer in biological systems-iron-sulphur proteins and cytochrome-C.

5.3. Magnesium (chlorophyll, photosystem-I and II), cobalt (vitamin B_{12}), zinc (carbonic anhydrase, carboxy peptidase and insulin).

BOOKS FOR STUDY:

1. Gurdeep Chatwal, Yadav, M.S., *Coordination Chemistry*, 1st Ed., Himalaya Publishing House, 1992.
2. Lasley Smart, Elain Moore, *Solid State Chemistry an Introduction*, 2nd Ed., Replica Press Pvt. Ltd. 2004.
3. Anthony R. West, *Solid State Chemistry and its Application*, 2nd Ed., John Wiley & Sons, 2014.
4. Huheey J. E., Keiter, E. A., Keiter, R. L., *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Ed., Harpercollins College Publishers, 1997.
5. Lee J.D., *Concise Inorganic Chemistry*, 5th Ed., Blackwell Science, 2015.
6. Asim K. Das, *Bioinorganic Chemistry*, Books and Allied Pvt. Ltd., Kolkata, Reprint 2011.
7. Kalsi P.S., Kalsi J.P., *Bioorganic, Bioinorganic and Supramolecular Chemistry*, 1st Ed., New Delhi, 2007.

BOOKS FOR REFERENCE:

1. Shriver, Atkins, *Inorganic Chemistry*, 4th Ed., Oxford University Press, 2006.
2. Cotton, F.A., Wilkinson, G., *Advanced Inorganic Chemistry*. 6th Ed., John Wiley & Sons, 1999.
3. Sathya Prakash, Tuli, G.D., Basu, S.K., Madan, R.D., *Advanced Inorganic Chemistry* 17th Ed., S. Chand & Co. Ltd., 1999.

WEB SOURCES:

1. https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Supplem

ental_Modules_(Inorganic_Chemistry)/Coordination_Chemistry/Structure_and_Nomenclature_of_Coordination_Compounds/Coordination_Number s_and_Geometry

2. https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Supplemental_Modules_(Inorganic_Chemistry)/Coordination_Chemistry/Complex_Ion_Equilibria/Complex-Ion_Equilibria
3. https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Supplemental_Modules_(Inorganic_Chemistry)/Coordination_Chemistry/Structure_and_Nomenclature_of_Coordination_Compounds/Coordination_Number s_and_Geometry
4. https://www.chemtube3d.com/category/inorganic-chemistry/advanced- solid-structures/
5. http://web.iitd.ac.in/~elias/links/Basic%20Inorganic%20chemistry%20part%203 Bioinorganic%20chemistry.pptx

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	identify the geometry of coordination compounds, examine the stereochemical aspects and stability of complexes	K4
CO2	analyze and explain the crystal field and molecular orbital theories of coordination compounds	K5
CO3	categorize and identify the structures and defects in solids and examine the electrical properties of solids	K4
CO4	classify HSAB and analyze the magnetic properties	K4
CO5	outline the role of metal ions and its complexes in biological systems	K2

K2-Understand; K4 – Analyze; K5 – Evaluate

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	M	S	L	-
CO2	S	M	S	S	M
CO3	S	M	S	S	S
CO4	S	M	S	S	-
CO5	S	-	S	M	-

S – Strong, M – Medium, L - Low

PROGRAMME TITLE : M.Sc. CHEMISTRY
COURSE TITLE : CORE-VIII : ORGANIC CHEMISTRY- II
COURSE CODE : 22PCHC5 HOURS/WEEK: 6 CREDITS: 5
SEMESTER : II

Course Objectives:

- To impart knowledge about elimination and addition reactions.
- To appreciate the reactivity of aromatic compounds.
- To get exposed to electrophilic substitution, molecular rearrangements, oxidation and reduction reactions and their application in synthesis.

Syllabus

UNIT-I **18 hours**

Elimination reactions

1.1 E1, E2 and E1CB mechanisms, orientation of double bond-Hofmann and Zaitsev's rule- Bredt's rule, molecular rearrangement during elimination, biological E1CB and E2 elimination reactions.

1.2 Pyrolytic elimination-mechanism and orientation- pyrolysis of esters of carboxylic acids. Effect of substrate structure, leaving group, attacking base and medium. Competition between substitution and elimination reactions.

1.3 Dehydration, dehydrohalogenation, Chugaev reaction, Hofmann degradation and Cope elimination.

UNIT-II **18 hours**

Addition to Carbon-Carbon and Carbon-Hetero Multiple Bonds

2.1 Mechanism of electrophilic addition-addition of halogen to olefin -stereochemistry of addition, addition of halogen in presence of water, addition of hydrogen halide to olefin-regiochemistry, Markovnikov and anti-Markovnikov addition, hydration of olefins-hydroboration/oxidation, oxymercuration-demercuration, acid catalysed hydration-stereochemistry of addition.

2.2 Hydroxylation of alkenes using OsO_4 and $KMnO_4$, Woodward and Prevost hydroxylation, Diels-Alder reaction-stereochemistry and regiochemistry, 1,3-dipolar addition reaction, addition of carbenes and nitrenes to double bond-singlet and triplet carbene- generation and their addition.

2.3 Mechanism of nucleophilic addition-reactions of carbonyl groups-Benzoin condensation, Mannich, Darzen, Wittig, Wadsworth-Emmons and Thorpe reactions.

UNIT-III **18 hours**

Electrophilic Substitution Reactions

3.1 Aromatic electrophilic substitution - arenium ion mechanism - orientation and reactivity in mono substituted benzene rings –ortho/para ratio- ipso attack – orientation in benzene rings with more than one substituent.

3.2 Formation of carbon–nitrogen σ-bond, nitration-applications, formation of carbon-halogen σ-bond-bromination, chlorination, iodination and fluorination, formation of carbon–sulphur σ-bond - sulphonation and chlorosulphonation - use of sulphonation and desulphonation reactions, formation of carbon–carbon σ-bond, Friedel–crafts alkylation and acylation, Houben–Hoesch reaction.

3.3 Formylation - Vilsmeier-Haack, Gattermann and Reimer-Tiemann reactions, Bischler – Napieralski, Hofmann Martius and Jacopsen reactions. Use of electrophilic aromatic substitution reactions in organic synthesis.

3.4 Aliphatic electrophilic substitution reactions SE1, SE2 front, SE2 back and SEi, Hell-Volhard-Zelinski reaction, Friedel- Crafts acylation at olefinic carbon, Stork-enamine reaction.

UNIT-IV **18 hours**

Molecular Rearrangements

4.1 Nucleophilic, electrophilic and free radical rearrangements-intramolecular and intermolecular rearrangements - migratory aptitudes - memory effects.

4.2 Wagner-Meerwin and related 1,2 shifts, Demyanov, Dienone-phenol, Favorski, Baeyer-Villiger, hydroperoxide, Stevens, Sommelet-Hauser, Smiles, Beckman, Hofmann, Baker-Venkatraman and Fries rearrangements.

UNIT-V **18 hours**

Oxidation and Reduction Reactions

5.1. **Oxidation**: Introduction- oxidation of alcohols to aldehydes and ketones using chromic acid, Jones reagent, Collins reagent, PCC, PDC, MnO_2 and silver carbonate, Swern oxidation - oxidative cleavage of glycols and related compounds - ozonolysis - Criegee mechanism, oxidation of methylene to carbonyl - oxidation of aryl methanes – oxidation of allylic and benzylic compounds- Etard reaction, oxidation of carbonyl compounds to 1,2-dicarbonyl compounds.

5.2 **Reduction:** Introduction- reduction of hydrocarbons-mechanisms and stereochemistry of catalytic hydrogenations- reduction of alkenes, alkynes and aromatic hydrocarbons, hydrogenolysis, heterogeneous and homogeneous hydrogenation-metal hydride reduction- Lithium aluminium hydride (LAH), Lithium tributoxyaluminiuim hydride, Sodium Boro Hydride ($NaBH_4$), $NaBH_3(CN)$, diborane, Birch reduction, Clemmensen reduction, Wolff-Kishner reduction, MPV reduction, Acyloin condensation.

BOOKS FOR STUDY:

1. Ahluwalia V. K., Parashar R. K., *Organic Reaction Mechanism*, 4th Ed., Narosa Publishing House, 2010.
2. Nimai Tewari, *Organic Chemistry - A Modern Approach*, Volume-II, McGraw Hill Education (India) Private Ltd., 2017.
3. Jagdamba Singh, Yadav L.D.S., *Advanced Organic Chemistry*, Pragati Prakashan, 8th Ed., 2012.
4. Smith M. B., Jerry March, *March's Advanced Organic Chemistry - Reactions, Mechanisms and Structure*, 6th Ed., John Wiley and Sons, 2007

BOOKS FOR REFERENCE:

1. Sanyal S. N., *Reactions, Rearrangements and Reagents*, Bharati Bhawan Publishers, 2019.
2. Jagdamba Singh, Yadav L.D.S., *Organic Synthesis*, Pragati Prakashan, 8th Ed., 2012.
3. Ratan Kumar Kar, *Applications of Redox and Reagents in Organic Synthesis*, Vol-I, New Central Book Agency Private Ltd., 2008.
4. Carruthers W., Iain Coldham, *Modern Methods of Organic Synthesis*, Cambridge University Press, 4th Ed., 2004.

WEB SOURCES:

1. https://epgp.inflibnet.ac.in/view_f.php?category=664
2. https://epgp.inflibnet.ac.in/view_f.php?category=660
3. https://www.masterorganicchemistry.com/2011/10/03/introduction -to-addition-reactions/
4. https://www.masterorganicchemistry.com/2013/03/22/hydroboratio n-of-alkenes/
5. https://www.masterorganicchemistry.com/2013/04/25/summaryalkene-reaction-pathways/

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	explain the concepts and factors affecting the reactions, the reactivity and orientation in aromatic electrophilic substitution	K4
CO2	explain the mechanism of elimination, addition, electrophilic substitution, molecular rearrangement, oxidation and reduction reactions	K3
CO3	predict the products of elimination, addition, electrophilic substitution, molecular rearrangement, oxidation and reduction reactions	K4
CO4	design synthetic route for unknown molecules using elimination, addition, electrophilic substitution, molecular rearrangement, oxidation and reduction reactions	K6
CO5	make use of appropriate reagents in organic synthesis and predict the stereochemistry and regiochemistry of products	K4

K3-Apply; K4-Analyse; K6-Create

Mapping of COs with POs

	POs				
COs	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**
CO1	S	M	S	S	M
CO2	S	S	S	S	M
CO3	S	M	S	S	S
CO4	S	M	S	S	S
CO5	S	S	S	S	M

S – Strong; M – Medium

Programme Title : M.Sc. CHEMISTRY

Course Title : ELECTIVE-II: CHEMICAL KINETICS AND THERMODYNAMCS

Course Code : 22PCHEC2 HOURS/WEEK: 6 CREDITS: 5

Semester : II

Course Objectives:

- *To learn about theories of reaction rates, kinetics of reactions in solution and irreversible thermodynamics*
- *To discuss the basic concepts of classical, quantum statistics and their applications*

Syllabus

UNIT-I **18 hours**

Chemical Kinetics -II

1.1. Kinetics of organic decomposition reactions - Rice-Herzfeld scheme – organic decomposition of ethane and acetaldehyde - chain length - kinetics of free radical polymerization reactions - pulse radiolysis.

1.2. Absolute reaction rate theory - thermodynamic terms - free energy, enthalpy and entropy of activation and their significance - partition functions and activated complex - Eyring equation - comparison of Eyring and Arrhenius equations.

1.3. Potential energy surfaces - dynamics of unimolecular reactions - Lindemann Hinshelwood, Rice-Ramsperger-Kassel (RRK) theory, Rice-Ramsperger- Kassel - Marsus (RRKM) theory.

UNIT II **18 hours**

Solution Kinetics

2.1 Ion transport in solutions - migration, diffusion, and convection - Fick's Laws of diffusion - reactions in solution, factors determining reaction rates in solutions, comparison between gas phase and solution reactions – cage effect.

2.2 Influence of solvent, ionic strength, and pressure on reactions in solution primary and secondary salt effect - Bronsted-Bjerrum equation – diffusion controlled reactions in solution - Debye–Smoluchowski equation

2.3 Kinetic isotope effects–effect of substituents on reaction rates - Hammett equation, Linear Free Energy Relationship - Taft equation - separation of polar, resonance and steric effects.

UNIT -III **18 hours**

Non-equilibrium thermodynamics

3.1. Basic concepts - forces and fluxes - entropy of irreversible processes- entropy production - Clausius inequality - phenomenological equations.

3.2. Onsager reciprocity relations coupled reactions, principle of microscopic reversibility, Onsager reciprocal relations – verification.

3.3. Entropy production- rate of entropy production, entropy production in chemical reactions – applications of irreversible thermodynamics to biological systems.

UNIT -IV **18 hours**

Statistical Thermodynamics-I

4.1 Objectives of statistical thermodynamics, concept of distributions, types of ensembles. thermodynamic probability, most probable distribution Law – classical statistics: Stirling's approximation formula, types of ensembles - Maxwell Boltzmann distribution law- assumptions and derivation.

4.2 Quantum statistics: Bose-Einstein and Fermi-Dirac statistics - comparison of Maxwell Boltzmann, Bose-Einstein and Fermi–Dirac statistics - entropy of boson - applications - derivation of Planck's black body radiation law, entropy of fermions, applications - electron gas, Fermi energy of free electrons at absolute zero.

UNIT -V **18 hours**

Statistical Thermodynamics-II

5.1 Definition and explanation - molecular partition function - molar partition function - derivation of thermodynamic quantities E, S, A, H, G, K and Cp, C_v using partition function.

5.2 Molar heat capacities of ideal gas molecules – translational, rotational, vibrational, and electronic partition functions - Sackur-Tetrode equation.

5.3 Equipartition principle of energy: calculation of heat capacities of ideal gases, Einstein and Debye theory of heat capacities of solids.

BOOKS FOR STUDY

1. Bajpai, D. N., *Advanced Physical Chemistry*, 2nd revised Ed., S. Chand & Company Ltd., 1998.
2. Keith. J. Laidler, *Chemical Kinetics*, 3rd Ed., Pearson education, New Delhi, 2007.
3. Puri L. R., Sharma Y. R., Pathania R. S., *Principles of Physical Chemistry*, 46th Ed., Vishal Publications, New Delhi, 2012.
4. Rajaram. J, Kuriacose J.C., *Chemical Thermodynamics*, 1st Ed., Pearson education, New Delhi, 2013.
5. Gurtu, J. N., Gurtu. A., *Advanced Physical Chemistry*, 25th Ed., Pragati Prakashan, Meerut, India, 2022.

BOOKS FOR REFERENCE

1. Atkins P.W., De Paula J., *Physical Chemistry*, 8th Ed., Oxford University Press, 2006.
2. McQuarrie D. A., *Text Book of Physical Chemistry*, University Science Books, Mill Valley, California, 1983.
3. Alberty R. A., Silbey, R. J., *Physical Chemistry*, John Wiley and Sons, New York, 1992.
4. Gasser R. P. H., Richards, W. G. *Introduction to Statistical Thermodynamics,* World Scientific Publishing Co. Pvt Ltd., Singapore, 1995.
5. Thomas Engel., Philip Reid., *Thermodynamics, Statistical Thermodynamics & Kinetics*, 3rd Ed., Pearson education, New Delhi, 2013.

WEB SOURCES:

1.http://staff.um.edu.mt/jgri1/teaching/che2372/notes/09/03/chain.html

2.https://www.educator.com/chemistry/physical-chemistry/hovasapian/statistical-thermodynamics_-the-various-partition-functions-i.php

3.https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Book%3A_Physical_Chemistry_(Fleming)/11%3A_Chemical_Kinetics_I

Course Outcomes

On the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	explicate the kinetics of chain reactions and comprehend the significance of theories of reaction rates	K4
CO2	examine the influence of physical parameters on reaction in solutions	K3
CO3	apply the concepts of irreversible thermodynamics to chemical reactions	K3
CO4	summarize the objectives, distribution law and applications of statistical thermodynamics	K4
CO5	calculate different partition function and know about theories of heat capacity	K3

K3-Apply, K4-Analyze

Mapping of COs with POs

	POs				
COs	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**
CO1	S	S	S	S	S
CO2	S	S	S	S	S
CO3	S	S	S	S	S
CO4	S	S	M	S	S
CO5	S	S	S	S	S

S – Strong; M – Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY
COURSE TITLE : ELECTIVE-II: GREEN CHEMISTRY
COURSE CODE : 22PCHESC2 HOURS/WEEK: 6 CREDITS: 5
SEMESTER : II

Course Objectives:

- *To learn about the green reagents and green synthesis*
- *To discuss about the aqueous phase reactions and organics synthesis in solid state*

SYLLABUS

UNIT – I **18 hours**

Green reagents and catalysts

DMC, polymer supported reagents, aid catalysts, oxidation catalysts, polymer supported catalysts, PTC, crown ethers, biocatalysts in organic synthesis - introduction - fermentation and bio transformations - production of bulk and fine chemicals by microbial fermentation. Antibiotics – vitamins - synthesis of industrial chemicals by bacterial constructs - future trends. Enzyme catalysed reactions, microbial oxidation and reduction.

UNIT – II **18 hours**

Microwave induced green synthesis

Microwave assisted reactions in water - Hofmann elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols. Microwave assisted reactions in organic solvents, solvent free reactions, ultrasound assisted green synthesis, saponification, substitution, coupling reactions, Friedel-Craft's reaction, Diels-Alder reaction, Cannnizaro reaction, Reformatsky reaction.

UNIT – III **18 hours**

Aqueous phase reactions

Diel's-Alder reactions, Claisen rearrangement, Aldol condensation, Knoevenegal reaction, Pinacol coupling, benzoin condensation, reduction of C=C, carbonyl compounds, aromatic compounds polymerisation, photochemical reactions, cycloaddition, electrochemical synthesis, adiponitrile, sebacic acid.

UNIT – IV **18 hours**

Green Synthesis

Green synthesis of the following compounds - adipic acid, catechol, disodium imino diacetate, a compostable and widely applicable plastic (poly lactic acid) made from corn.

Organic synthesis in solid state - Michael addition, nuclear halogenation, Grignard reaction, nitration, Beckmann rearrangement, dimerisation of fullerene, synthesis of β-lactam, aziridines and quinoline.

Unit V **18 hours**

Greener synthesis of nanoparticles

Physical synthesis of nanoparticles – inert gas condensation - aerosol method - arc discharge - laser ablation - gas-phase synthesis – chemical synthesis of nanoparticles – precipitation and co-precipitation method, sol-gel method, solvothermal and hydrothermal method, chemical vapour synthesis.

BOOKS FOR STUDY:

1. Ahluwalia, V. K., Kidwai, M., *New Trends in Green Chemistry*, Reprint, Springer

Publishers, 2012.
2. Sanghi, R., Srivastava, M. M., *Green Chemistry*, Reprint, Narosa Publishing House, New Delhi, 2012.
3. Bandyopadhyay. C., *An insight into Green Chemistry*, 1st Ed., Books & Allied Pvt. Ltd., 2019.

BOOKS FOR REFERENCE:

1. Ahluwalia, V.K., *Green Chemistry*, 2nd Ed., Ane Books Pvt. Ltd., 2017.
2. Ahluwalia, V.K., *Strategies for Green Organic Synthesis*, 1st Ed., Ane Books Pvt. Ltd., 2012.

WEB SOURCES:

1. https://www.epa.gov/greenchemistry/basics-green-chemistry
2. https://www.researchgate.net/publication/308995209_the_role_of_catalysts_in_green_synthesis_of_chemicals_for_sustainab le_future
3. https://www.researchgate.net/publication/261872979_Microwave_assisted_synthesis_a_green_chemistry_approach

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	compare various green reagents, catalysts and their utility	K2
CO2	explain the significance of microwave induced green synthesis	K3
CO3	apply the aqueous phase reactions in experiments	K3
CO4	synthesize organic compounds using greener methods	K6
CO5	illustrate about the greener synthesis of nanoparticles	K2

K2-Understand; K3-Apply; K6-Create

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	M	S	S	S
CO2	S	S	S	S	S
CO3	S	S	S	S	S
CO4	S	S	S	S	S
CO5	S	S	S	S	S

S-Strong; M-Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY
COURSE TITLE : CORE-IV: INORGANIC CHEMISTRY PRACTICAL
COURSE CODE : 22PCHQC1 HOURS/WEEK: 3 (I Sem.) + 3 (II Sem.)
SEMESTER : I & II CREDITS: 3

Course objectives

- *To stimulate the interest in the field of qualitative analysis and to understand the reactivity of common and rare earth cations.*
- *To learn about photocalorimetric, cerimetric and complexometric titrations.*

SYLLABUS

1. Qualitative analysis:

Semi-micro qualitative analysis of mixture containing two common and two rare cations. The following rare cations to be included: W, Se, Te, Ce, Th, Ti, Zr, V, Be, U and Li.

2. Quantitative analysis:

2.1. Complexometric titrations: Estimations of Zn, Ca, Mg, Ni and Hardness of water.

2.2. Cerimetry: Cerimetric estimation of Fe (II) and oxalic acid

3. Demonstration experiments:

3.1. Photocolourimetry- Estimation of Fe, Ni, Mn, Ti and Co (II)

3.2. Flame photometry-Estimation of Na and K

3.3. Estimation of Iron in Iron tablets

3.4. Estimation of Ca in calcium tablets

BOOKS FOR REFERENCE:

1. Venkateswaran, V., Veeraswamy, R., Kulandaivelu, A.R., *Basic Principles of Practical Chemistry*, 2nd Ed., S. Chand & Sons, 1997.
2. Ramanujam, V. V., *Inorganic Semi Micro Qualitative Analysis*, 3rd Ed., The National Publishing Co., 1990.

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	demonstrate the basic principles of qualitative inorganic analysis	K2
CO2	identify various rare and common cations present in inorganic mixture	K3
CO3	analyze the rare earth elements qualitatively	K4
CO4	determine the strength of Fe, Ni, Mn, Ti, Co(II) by photocolorimetry and Na, K by flame photometry	K5
CO5	estimate the amount of ions by complexometric and cerimetric titrations	K6

K2 – Understand; K3 – Apply; K4 - Analyze; K5 – Evaluate; K6- Create

Mapping of COs with POs

COs	POs				
	PO1	**PO2**	**PO3**	**PO4**	**PO5**
CO1	M	M	M	M	M
CO2	M	S	S	M	M
CO3	S	S	S	S	S
CO4	S	S	S	S	S
CO5	S	S	S	S	S

S – Strong; M – Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY
COURSE TITLE : CORE-V: ORGANIC CHEMISTRY PRACTICAL-I
COURSE CODE : 22PCHQC2 HOURS/WEEK: 3 (I Sem.) + 3 (II Sem.)
SEMESTER : I & II CREDITS: 3

Course Objectives:

- To familiarize the students with estimation of organic compounds like phenol, aniline etc.
- To train students in the synthesis of organic compounds
- To learn the analytical techniques such as chromatography

Syllabus

Organic estimations

1. Phenol
2. Aniline
3. Methyl ketone
4. Glucose
5. Carboxylic acid/Ascorbic acid
6. Iodine value of an oil
7. Saponification value of an oil

Organic preparations involving two stages

1. Sym-tribromobenzene from aniline
2. 5-Nitrosalicylic acid from methyl salicylate
3. Aspirin from methyl salicylate
4. Bezanilide from benzophenone

Organic preparations involving three stages

5. *p*-Nitroaniline from acetanilide/aniline
6. *p*-Bromoaniline from acetanilide/aniline

Extraction of natural products

1. Citric acid from lemon/pineapple
2. Caffeine from tea leaves
3. Curcumin from turmeric
4. Lactose from milk

Chromatographic separations

1. TLC - separation of a mixture of two or more organic compounds.
2. Paper chromatography - identification of natural amino acids.
3. Column chromatography - separation of a mixture of *o* & *p*-nitroaniline.

Microwave assisted synthesis of organic compounds

1. Heterocyclic compounds
2. Chalcones

BOOKS FOR REFERENCE:

1. Pavia, D. L., Lampman, G. M., Kris, G. S., Engel, R. G., *A Micro Scale Approach to Organic Laboratory Techniques,* 6th Ed., Cengage Learning, 2016.
2. Zubrick., J. W., *The Organic Chem Lab Survival Manual: A Student's Guide to Techniques,* 9th Ed., John Wiley & Sons, 2014.
3. Gnanaprakasam, N.S., Ramamurthy, G., *Organic Chemistry Lab Manual*, S. Viswanathan Printers and Publishers Private Ltd. 2002.

4. Raj K. Bansal, *Laboratory Manual of Organic Chemistry*, 5th Ed., New Age International (P) Ltd., 2009.
5. Vishnoi, N.K., *Advanced Practical Organic Chemistry*, Vikas Publishing House Pvt. Ltd., 2nd Reprint, 1994.

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	identify limiting reagents, calculate the theoretical & percentage yield and perform experiments safely	K3
CO2	develop skills in the greener synthesis of organic compounds and laboratory techniques including distillation, recrystallization and chromatography	K3
CO3	utilize extraction techniques for the preparation of organic compounds from natural products	K3
CO4	explain the theory behind the experiments performed and give a detailed mechanism for all laboratory reactions	K5
CO5	estimate organic compounds volumetrically	K6

K3 – Apply; K5 – Evaluate; K6- Create

Mapping of COs with POs

	POs				
COs	PO1	PO2	PO3	PO4	PO5
CO1	M	S	S	S	S
CO2	M	S	S	S	S
CO3	M	S	S	S	S
CO4	S	S	M	S	S
CO5	M	S	S	S	S

S – Strong; M – Medium

Programme Title : M.Sc. CHEMISTRY
Course Title : CORE-VI: PHYSICAL CHEMISTRY PRACTICAL- I
Course Code : 22PCHQC3 HOURS/WEEK: 3 (I Sem.) + 4 (II Sem.)
Semester : I & II CREDITS: 3

Course Objectives:

- *To develop skill, practical knowledge about potentiometric experiments, adsorption isotherms and to impart knowledge about phase diagrams*

Syllabus

Phase rule

1) Two component systems-simple eutectic system-construction of phase diagram for a simple binary system (naphthalene-biphenyl or benzophenone- diphenyl amine)

Potentiometry

2) Strong acid Vs strong base (HCl Vs NaOH).
3) Weak acid Vs strong base (CH_3COOH Vs NaOH).
4) Mixture of acids Vs strong base (CH_3COOH+HCl Vs NaOH).

Precipitation titrations

5) Sodium chloride Vs silver nitrate
6) Potassium iodide Vs silver nitrate
7) Potassium bromide Vs silver nitrate
8) Mixture of halides Vs silver nitrate.

Redox titrations

9) Ferrous ions Vs potassium permanganate.
10) Ferrous ions Vs potassium dichromate.
11) Ferrous ions Vs ceric ammonium nitrate
12) Potassium iodide Vs potassium permanganate.

Adsorption

13) To investigate the adsorption of oxalic acid from aqueous solution by activated charcoal, determination of surface area and examine the validity of Freundlich and Langmuir's adsorption isotherms.
14) To determine the adsorption isotherms of acetic acid from aqueous solutions by charcoal.
15) To study the adsorption of I_2 from alcoholic solution by charcoal.

Miscellaneous

15) Determination of pH of buffer solution – quinhydrone electrode.
16) Determination of solubility, solubility product of AgI - half cell method, concentration method.
17) Determination of dissociation constant of a weak acid.
18) Determination of activity coefficient of Ag^+ ions using concentration cell with salt bridge.
19) Determination of transport number of Ag^+ and NO_3^- ions.
20) Determination of single electrode potentials (Ag/Ag^+, Zn/Zn^{2+}, Cu/Cu^{2+}).

Demonstration experiment:

Two component systems - compound formation with congruent melting point.

BOOKS FOR REFERENCE

1. Viswanathan, B., Raghavan, P.S., *Practical Physical Chemistry*, 1st Ed., Viva Books Pvt. Ltd., 2005.
2. Levitt, B.P., *Findlay's Practical Physical Chemistry*, 9th Ed., Longman Group Ltd., 1973.
3. Yadav, J. B., *Advanced Practical Physical Chemistry*, 27th Ed., Goel Publishing House, 2008.

Course Outcomes

On the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	construct and analyse the phase diagram to determine the eutectic point	K3
CO2	develop skills in the potentiometric estimation of acid-base, precipitation and redox titrations	K2
CO3	Evaluate normality and pH of various solutions	K3
CO4	determine the solubility of sparingly soluble salts	K3
CO5	interpret Freundlich and Langmuir Adsorption isotherms	K3

K2-Understand; K3-Apply

Mapping of COs with POs

	POs				
COs	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**
CO1	S	S	S	S	S
CO2	S	S	S	S	S
CO3	S	S	S	S	S
CO4	S	S	M	S	S
CO5	S	S	S	S	S

S – Strong; M – Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : CORE-IX: ORGANIC CHEMISTRY-III

COURSE CODE : 22PCHC6 HOURS/WEEK: 5 CREDITS: 4

SEMESTER : III

Course Objectives:

- *To learn the basic concepts of aromaticity and retro synthesis and their applications.*
- *To understand the concept of method of designing an organic synthesis using various reagents in synthetic organic chemistry.*
- *To know the synthesis and properties of heterocyclic compounds.*
- *To get an insight of natural products and synthesis of alkaloids, terpenoids, carotenoids and steroids.*

SYLLABUS

UNIT-I 15 Hours

Aromaticity and Retro Synthesis

1.1 Aromaticity

Criteria - Huckel's rule – Aromatic character in benzene, four, five, seven, eight membered rings- Aromaticity of benzenoids and heterocyclic compounds. Non-benzenoid aromatics-azulene, ferrocene, tropolone, sydnones and annulenes (synthesis not required) – Non-aromatic and anti-aromatic systems.

1.2 Retro synthesis

Definitions of some terms used in retro synthesis- Guidelines for choosing disconnections - Guidelines - 1 to 3. One group C-X disconnections- carbonyl derivatives, alcohols and olefins.

1.3. Chemoselectivity - Introduction, Guidelines-1 to 7. Reversal of polarity (Umpolung) – Definition- Umpolung reagents (Epoxides, α – halo ketones, nitro compounds).

UNIT-II 15 Hours

Protecting Groups and Reagents in Organic Synthesis

2.1 Protecting Groups - Introduction, protection of alcohols- principle –protecting group for alcohols- acetals/ketals, ethers, protection of carbonyl groups- principle – protecting group for carbonyl compounds- acyclic acetals and ketals.

2.2 Protection of carboxylic acid groups- principle – protecting group for carboxylic acid – methyl ester, protection of amino groups- principle – protecting group for amino group- formamide.

2.3 Reagents in organic synthesis - use of the following reagents in organic synthesis and functional group transformation – lithium dimethyl cuprate (LDC), lithium diisopropyl amide (LDA), dicyclohexyl carbodimide (DCC),1,3 –Dithiane (reaction umpolung), trimethyl silyl iodide, diisobutyl aluminium hydride (DIBAL-H), DDQ, Baker's yeast.

UNIT–III **15 Hours**

Heterocyclic compounds

3.1 Synthesis and properties of imidazole, oxazole & thiazole. Structural elucidation and synthesis of anthocyanidins - Cyanin chloride, Pelargonin chloride, Delphinin chloride & Peonin chloride.

3.2 Synthesis and structural elucidation of flavones, isoflavones & flavanols-Diadzein, Quercetin.

3.3 Synthesis of pyrimidine and its derivatives-synthesis of uric acid, purine and its derivatives.

UNIT–IV **15 Hours**

Alkaloids, Terpenoids and Carotenoids

4.1 Alkaloids - synthesis and structural elucidation of quinine, morphine and reserpine.

4.2 Terpenoids - biosynthesis of alkaloids and terpernoids (elementary treatment only)-chemistry of juvenile hormone, abietic acid, squalene .

4.3 Carotenoids - α, β, γ - carotenoids-lycopene-Vitamin A_1.

UNIT–V **15 Hours**

Steroids

5.1 Structure and stereochemistry of cholesterol, ergosterol, oestrone, cortisone.

5.2 Application of ORD and CD, detection of absolute configuration, octant rule, cotton effect-axial haloketone rule for cholesterol.

5.3 Conversion of cholesterol to progesterone, testosterone and oestrone – conversion of ergosterol to progesterone.

BOOKS FOR STUDY:

1. Jerry March, *Advanced Organic Chemistry Reactions Mechanisms and Structure*, 4th Ed., John Wiley and Sons, 2003.
2. Paula Yurkanis Bruice, *Organic Chemistry*, 8th Ed., Pearson, 2016.
3. Jagadamba Singh & Yadav, L.D.S., *Advanced Organic Chemistry*, 6th Ed., Pragati Prakasam, 2007.

4. Ratan Kumar Kar, *Fundamentals of Organic Synthesis* – Vol II, Revised Ed., New Central Book Agency Pvt. Ltd. Kolkata, 2008.
5. Stuart Warren, *Organic Synthesis- The Disconnection Approach*, 1st Ed., John Wiley, New York, 2004.
6. Finar, I.L., *Organic Chemistry*, Vol II, 5th Ed., ELBS, 2011.

BOOKS FOR REFERENCE:

1. Ahluwalia, V.K., *Organic Reaction Mechanism*, 4th Ed., Narosa Publishing House, 2013.
2. Mukherji, S. M. & Singh, S.P., *Reaction Mechanism in Organic Chemistry*, 1st Ed., The Macmillan Company of India Ltd. 1984.
3. Carey, F.A. & Sundberg, R.J., *Advanced Organic Chemistry*, Part A, Springer Science Business Media, LLC, 2007.
4. Gurdeep K. Chatwal, *Organic Chemistry of Natural Products*, Vol. II, 5th Ed., Himalaya Publishing House, 2013.

WEB SOURCES:

1. https://www.pharmatutor.org/articles/imidazole-synthesis-properties-biological-activity
2. http://www.chem.ucla.edu/~harding/tutorials/carbos/representations.df
3. http://renaud.dcb.unibe.ch/topic-review/topic-review-2012/tr2012_05-morphine.pdf
4. https://en.wikibooks.org/wiki/Structural_Biochemistry/Lipids/Cholestel
5. https://www.tcichemicals.com/pdf/ReagentGuide_8th_SynthesticOrganicChemistry_MaterialsChemistry.pdf

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	classify organic compounds as aromatic/non-aromatic and antiaromatic	K4
CO2	apply retero synthesis for designing different synthetic routes	K3
CO3	plan the use of protecting groups and reagents in synthetic organic chemistry	K3
CO4	analyse the structure of heterocycles and natural products	K4
CO5	plan the synthesis and identify the properties of heterocycles and natural products	K3

K3-Apply; K4-Analyse

Mapping of COs with POs

COs	POs				
	PO1	**PO2**	**PO3**	**PO4**	**PO5**
CO1	S	-	S	S	S
CO2	S	M	S	S	S
CO3	S	M	S	S	S
CO4	S	-	S	S	S
CO5	S	L	S	S	S

S- Strong; M- Medium; L- Low

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : CORE-X: PHYSICAL CHEMISTRY-II

COURSE CODE : 22PCHC7 HOURS/WEEK: 5 CREDITS: 4

SEMESTER : III

Course Objectives:

- *To enrich the understanding of various photophysical processes and significance of solar energy conversion.*
- *To learn about the latest advances and trends in applied electrochemistry.*
- *To gain knowledge about electrodics in biology and environmental science.*

SYLLABUS

UNIT-I 15 Hours

Photophysical Chemistry

1.1 Electronic transitions and intensity of absorption bands; excited state kinetics - electronic energy transfer mechanism-excimer and exciplex .

1.2 Kinetics of luminescence- phosphorescence- fluorescence-quenching mechanism - Stern-Volmer equation- kinetics of photosensitized reactions and photodissociation reactions .

1.3 Fabrication of photovoltaic and photogalvanic cells for solar energy conversion – current scenario in solar thermal power generation

UNIT-II 15 Hours

Surface chemistry and catalysis

2.1 Kinetics of surface reactions-physical and chemical adsorption-adsorption isotherms- types of adsorption isotherms.

2.2 Langmuir adsorption isotherm-B.E.T theory for multilayer adsorption. Application of transition state theory to adsorption measurement of surface area-mechanism of heterogeneous catalytic reactions.

2.3 Acid base catalysis-mechanism-Bronsted catalysis law-catalysis by enzymes-rate of enzyme catalysed reactions-effect of substrate concentration, pH and temperature on enzyme catalyzed reactions-inhibition of enzyme catalyzed reactions.

UNIT-III **15 Hours**

Electrochemistry-I

3.1 Debye-Huckel theory of strong electrolytes – Debye-Huckel-Onsager equation-verification -conductivity at high field and at high frequency-Debye-Huckel limiting law and its extension – Bjerrum ion pair theory.

3.2 Electrode - Electrolyte interface - adsorption at electrified interface-electrical double layer-electro capillary phenomena, Lippmann equation.

3.3 Structure of electrical double layer-Helmholtz -Perrin, Gouy-Chapman and Stern models.

UNIT-IV **15 Hours**

Electrochemistry-II

4.1 Electrodics-mechanism of electrode reactions- over potential- Butler-Volmer equation for one step one electron transfer reactions—Tafel equation- significance of equilibrium exchange current density-mechanism of hydrogen, oxygen evolution reactions.

4.2 Prevention of corrosion –proper designing and material selection, cathdoic protection, protective coatings, metal cladding and spraying, hot dipping, anodic and cathodic inhibitors-construction of Pourbaix and Evans diagrams.

4.3 Energy storage devices – nickel-cadmium, Zn-O_2, and Lithium ion batteries - capacitors and super capacitors.

UNIT-V **15 Hours**

Electrodics in Biology and Environmental Remediation

5.1 Bioelectrodics - Diffusion potential - Donnan membrane equilibrium-Bioelectrochemistry of excitable cells (nerve cells) – electrical conductivity in biological organisms- spike potential- enzymes as electrodes.

5.2 Electrochemical technology in pollution control - process handling of waste-electroplating-electrochemical transport system – electrochemical engine - electric vehicles.

5.3 Need for photoelectrocatalysis -photoelectrochemical splitting of water-photoelectrochemical decomposition of H_2S.

BOOKS FOR STUDY:

1. Atkins, P.W., & Julio de Paulo, *Atkins' Physical Chemistry*, 10th Ed., Oxford University Press, 2014.

2. Rohatgi, K.K., & Mukherjee, *Fundamentals of Photochemistry*, 3rd Ed., New Age International (P) Publishers, 2017.
3. Bajpai, D.N., *Advanced Physical Chemistry*, 2nd Ed., S. Chand & Company Ltd., 2015.
4. Glassstone, S., *Introduction to Electrochemistry*, 10th Ed., Affiliated East West Press, 2007.

BOOKS FOR REFERENCE:

1. Laidler, K.J., *Chemical Kinetics*, 3rd Ed., Pearson Education Inc., 2007.
2. Bockris, J.O.M., & Reddy A.K.N., *Modern Electrochemistry*, Volumes 2A & 2B, 2nd Ed., Kluwer Academic Publishers, 2004.

WEB SOURCES:

1. https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Book%3A_Physical_Chemistry_(Fleming)/11%3A_Chemical_Kinetics_I
2. https://nptel.ac.in/courses/104/106/104106129/
3. https://nptel.ac.in/courses/103/108/103108162/

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	utilize the concepts of photochemical and catalytic reactions to various applications	K3
CO2	distinguish between different theories of adsorption and homogeneous catalysis	K4
CO3	analyse the kinetics of photochemical and catalytic reactions	K4
CO4	assess the nature of electrolytes and electrode-electrolyte interface models	K5
CO5	discuss the applications of electrodics in material science, energy storage devices, biology and environmental remediation	K5

K3-Apply; K4-Analyse; K5-Evaluate

Mapping of COs with POs

COs	POs				
	PO1	**PO2**	**PO3**	**PO4**	**PO5**
CO1	S	S	S	S	S
CO2	S	S	M	S	S
CO3	S	S	S	S	S
CO4	S	S	S	S	S
CO5	S	M	S	S	S

S- Strong; M- Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : CORE-XI: COORDINATION CHEMISTRY

COURSE CODE : 22PCHC8 HOURS/WEEK: 5 CREDITS: 4

SEMESTER : III

Course objectives

- *To gain knowledge on different term states in different ligand fields.*
- *To understand the electronic spectra of complexes.*
- *To know about the substitution reaction mechanisms.*
- *To discuss the bonding involved in organometallic compounds and its applications*.

SYLLABUS

UNIT- I **15 Hours**

Electronic spectra of complexes

1.1. Spectroscopic term symbols for d^n ions-derivation of term symbols and ground state term symbol.

1.2. Selection rules-breakdown of selection rules, Spin-orbit coupling, band intensities, weak and strong field limit.

1.3. Energy level diagrams - Orgel and Tanabe-Sugano diagrams, effect of distortion and spin-orbit coupling on spectra, evaluation of D_q and B values for octahedral complexes of nickel.

1.4. Charge transfer spectra.

1.5. Spectral and magnetic properties of lanthanides.

UNIT-II **15 Hours**

Reaction mechanism in octahedral complexes.

2.1. Discussion of A, D, Ia, Id and DcB mechanism, evidence for conjugate base mechanism.

2.2. Replacement of coordinated water, mechanism of acid and base hydrolysis.

2.3. Template reactions, rearrangement reactions in four coordinate and six coordinate complexes.

2.4. Synthesis of platinum and cobalt complexes.

UNIT-III **15 Hours**

Magnetic properties and Bio-medical applications of complexes

3.1. Magnetic properties of metal complexes: origin of magnetic behaviour, dia, para, ferro and anti-ferro magnetism, calculation of magnetic moment, magnetic properties of A, E and T ground terms in complexes, quenching of orbital magnetic moment by crystal field, spin-orbit coupling, spin-crossover in coordination compounds.

3.2. Bio-medical applications: role of metal complexes -cisplatin as anticancer agent, anticancer activity of rhodium, gold, copper, and cobalt complexes. Detoxifications of metals using chelating agents-complexation of food poisoning.

UNIT-IV **15 Hours**

Organometallic chemistry

4.1. Introduction and classification of organometallic compounds by bond types viz. covalent, ionic, electron deficient and cluster compounds, nomenclature, ligand hapticity, electron count for different types of organometallic compounds, the 18-electron rule and 16-electron rule.

4.2. Synthesis, properties and pi-bonding of organometallic complexes of alkenes, alkynes, allyl, & pentadienyl (metallocene) complexes, Davis-Green-Mingos (DGM) rules.

4.3. Metal-metal bonds- EAN rule, -framework bonding in metal clusters, type of clusters viz. carbonyl cluster, halide clusters and hydrido clusters, electron counting in medium size cluster (Wade's rule, Capping rule), cluster of Fe, Ru, Os groups. Cluster of Co, Rh, Ir groups. Cluster of Ni, Pd, Pt groups.

UNIT-V **15 Hours**

Industrial application of organometallic compounds

5.1. Oxidative addition and reductive elimination in organometallics.

5.2. Fluxional isomerism.

5.3. Hydrogenation of olefins (Wilkinson catalyst).

5.4. Oxo process (Co and Rh catalyst), oxidation of olefins to aldehydes and ketones (Wacker's process).

5.5. Polymerisation (Ziegler –Natta Catalyst), cyclo-oligomerisation of acetylene using Ni catalyst (Reppe's catalyst); polymer bound catalyst.

BOOKS FOR STUDY:

1. Gopalan, R., Ramalingam V., *Concise Coordination Chemistry*, 1st Ed., Vikas Publication House Pvt. Ltd., 2001.
2. Puri, B.R., Sharma, L.R., Kalia, K.C., *Principles of Inorganic Chemistry*, 33rd Ed., Vishal Publishing Co., Delhi, 2016.
3. Gary L. Miessler, & Donald A. Tarr, *Inorganic Chemistry*, 3rdEd., Dorling Kindersley (India) Pvt. Ltd., 2009.
4. Mehrotra, R.C., & Singh, A., *Organometallic Chemistry-A Unified Approach*. New Age International (P) Ltd., 1st Ed., 2009.

BOOKS FOR REFERENCE:

1. Drago, R.S., *Physical Methods in Chemistry*, Reinhold New York, 1st Ed., 1968.
2. Shriver, D.F., Atkins, P.W., & Longford, C.H., *Inorganic Chemistry*, 4th Ed., ELBS, 2006.
3. Huheey, J.E., Keiter E.A., & Keiter, L., *Inorganic Chemistry – Principles of Structure and Reactivity*, 4th Ed., Pearson Education, 1997.

WEB SOURCES:

1. https://www.dalalinstitute.com/books/a-textbook-of-inorganic-chemistry-volume-1/electronic-spectra-of-transition-metal-complexes/
2. https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Book%3A_Inorganic_Chemistry_(Saito)/6%3A_Chemistry_of_Transition_Metals/6.4%3A_Reactions_of_Complexes
3. https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Supplemental_Modules(Inorganic
4. Chemistry/Organometallic_Chemistry/Fundamentals_of_Organometallic_Chemistry/Associative_Ligand_Substitution
5. https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Supplemental_Modules(Inorganic_Chemistry)/Organometallic_Chemistry/Fundamentals_of_Organometalli_Chemistry/Dissociative_Ligand_Substitution_Reactions
6. https://nptel.ac.in/content/storage2/nptel_data3/html/mhrd/ict/text/104108062/lec29.pdf
7. https://www.chemtube3d.com/oxo_reaction/

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	apply the concepts of electronic spectra of transition metals and predict the ground state and excited state terms symbols	K6
CO2	analyze the reaction mechanism of octahedral complexes and interpret the rate of electron transfer reactions	K4
CO3	evaluate the magnetic behaviour of complexes and explain the biomedical applications of metal complexes	K5
CO4	classify the structure and bonding aspects of organometallic compounds and predict their shape and geometry	K6
CO5	explain the general idea of catalysis and analyse the various organometallic catalyst mechanisms	K4

K4-Analyse; K5 – Evaluate; K6 - Create

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	S	S	M	-
CO2	S	S	S	S	-
CO3	S	M	S	S	S
CO4	S	S	S	S	S
CO5	S	S	S	S	S

S-Strong; M-Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : ELECTIVE – III: GROUP THEORY AND SPECTROSCOPY

COURSE CODE : 22PCHEC3 HOURS/WEEK: 5 CREDITS: 4

SEMESTER : III

Course Objectives:

- *To comprehend the concepts of symmetry.*
- *To derive spectral activity and hybridization based on symmetry considerations.*
- *To understand the elementary concept of SALCS in explaining MOs.*
- *To have an overview of theory and principles of spectroscopic techniques such as microwave, NQR, IR, Raman, UV- Visible.*

SYLLABUS

UNIT-I 15 Hours

Introduction to Chemical Groups

1.1. Definition of Group-basic properties of group-symmetry elements and symmetry operation, Symmetry criteria for optical activity, symmetry and dipole moment, symmetry and stereo isomerism, symmetry classification into point groups (schoenflies symbol only), determination of point groups.

1.2. Abelian group-cyclic group-sub group-isomorphic group-similarity transformation and classes-group multiplication tables.

1.3. Matrices: Types of matrices- rectangular, square, column, row, diagonal, scalar, unit, matrix notation for symmetry elements, matrix representation of C_{2V} and C_{3v} point group, character of a representation-character of a matrix, characters of conjugate matrices.

UNIT- II 15 Hours

GOT and Character Table

2.1. Definition of reducible and irreducible representations – irreducible representations as orthogonal vectors- rule- the great orthogonality theorem (GOT) and its consequences (statement only, proof not needed).

2.2. Construction of character tables (C_{2V} and C_{3V} point groups) using orthogonality theorem, properties of irreducible representation, Mulliken symbols for irreducible representations, calculation of translational, rotational and binary co-ordinates in the

character tables for C_{2V} and C_{3V} point groups, relation between reducible and irreducible representation-reduction formula, direct product of representations-problems involving direct product of IRs.

2.3. **Group theory and vibrational spectroscopy**: vibrational modes as basis for group representation-symmetry selection rules for IR and Raman spectra-mutual exclusion principle- determination of representation of vibrational modes in non-linear molecules and determine the Raman and IR activity of their vibrations-C_{2v} molecules like-H_2O, SO_2, Cl_2O, ClF_3, cis-N_2F_2, cis-$[PtCl_2X_2]$, C_{3v} molecules namely NH_3, $POCl_3$, fac-ML_3X_3, D_{2h}-Ethene and D_{4h}-XeF_4, symmetry requirements for overtones and combination bands.

UNIT-III **15 Hours**

Applications of Group Theory

3.1. Applications of direct product, symmetry adapted linear combinations, bonding in polyatomics.

3.2 Constructing molecular orbitals and hybrid orbitals from SALCs, criteria of overlap in LCAO approximation, designation and symmetry of MOs, modes of overlap of AOs .

3.3. Application of group theory in determining hybridization –hybrid orbitals of sigma bonding-T_d, D_{3h}, D_{4h} and C_{4v} molecules

UNIT-IV **15 Hours**

Nuclear Quadrupole Resonance and Microwave Spectroscopy

4.1. Nuclear quadrupole resonance-theory-applications of NQR-(nature of chemical bond-study of chloromethanes, chloroacetyl chlorides, structural information about the group III halides, study of charge transfer compounds).

4.2. Microwave spectroscopy-theory –rotation of molecules-rotational spectra of diatomic molecules –rigid rotator, non-rigid rotator –intensity of spectral lines-effect of isotopic substitution-Stark effect (derivation not needed)-application of microwave spectroscopy.

UNIT-V **15 Hours**

Vibrational and UV Spectroscopy

5.1. IR spectroscopy-basic principles- harmonic oscillator-anharmonic oscillator-vibrating rotator –linear molecules(PR and PQR branch lines) –fundamental, overtone, combination, difference bands and hot bands-Fermi resonance- IR spectra of

polyatomic molecules (H_2O and CO_2) –factors affecting vibrational frequencies – finger print region

5.2. Raman spectroscopy-Raman effect-Raman scattering Vs Rayleigh scattering, Raman Vs fluorescent scattering, Raman lines and Raman frequencies, Theory of Raman effect, polarization of Raman lines, condition for Raman activity, complementary nature of IR and Raman spectroscopy, intensity of Raman lines, rotational Raman spectra, vibrational Raman spectra, vibration-rotational Raman, Resonance Raman spectroscopy and coherence anti-stokes Raman spectroscopy

5.3. Electronic spectra of diatomic molecules-vibrational coarse structure-Franck-Condon principle-dissociation energy and dissociation products-predissociation-Birge spooner method of evaluation of dissociation energy from electronic spectra-rotational fine structure of electronic vibrational transitions.

BOOKS FOR STUDY:

1. Veera Reddy, K., *Symmetry and Spectroscopy of Molecules*, 2nd Ed., New Age International Ltd., 2009.
2. Cotton, F.A., *Chemical Applications of Group Theory*, 3rd Ed., John Wiley and Sons Inc., New York,1972.
3. Banwell, C.N., *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata McGraw Hill Publishing Company Limited, New Delhi, 2008.

BOOKS FOR REFERENCE:

1. Bhattacharya, P.K., *Group Theory and its Chemical Applications*, 2nd Ed., Himalaya Publishing House, 2020.
2. Alan Vincent., *Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications*, 2nd Ed., Wiley, 2001.
3. Chatwal, G.R., & Anand, S.A., *Instrumental Methods of Chemical Analysis,* 5th Ed., Himalaya Publishing House, Mumbai, 2007.

WEB SOURCES:

1. https://onlinecourses.nptel.ac.in/noc21_cy16/preview
2. http://vallance.chem.ox.ac.uk/pdfs/SymmetryLectureNotes.pdf
3. https://vlab.amrita.edu/?sub=2
4. https://chem.libretexts.org

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	explain the principles of symmetry of molecular groups, matrices and the concepts underlying the microwave, NQR, IR, Raman and electronic spectroscopy	K2
CO2	identify and determine the point groups of molecules and hybridisation	K5
CO3	predict the IR - Raman activity of molecular vibrations using character tables	K6
CO4	construct C_2v, C_3v character table and MOs using LCAO and explain the application of group theory in determining hybridisation	K3
CO5	solve the problems relating to structure determination involving microwave spectroscopy and IR spectroscopy	K6

K2-Understand; K3-Apply; K5-Evaluate; K6-Create

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	-	S	M	M
CO2	S	-	S	M	S
CO3	S	S	S	M	M
CO4	S	L	M	S	S
CO5	S	S	M	S	S

S-Strong; M-Medium; L-Low

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : ELECTIVE – III: NANOCHEMISTRY

COURSE CODE : 22PCHESC3 HOURS/WEEK: 5 CREDITS: 4

SEMESTER : III

Course Objectives:

- *To know the synthetic methods of nanomaterials.*
- *To understand the characterization of nanomaterials.*
- *To understand carbon clusters and nanostructures.*
- *To learn nanotechnology and nanodevices.*

SYLLABUS

UNIT- I **15 Hours**

Synthetic Methods

1.1 Definition of nanodimensional materials – historical milestones – unique properties due to nanosize, quantum dots, classification of nanomaterials. General methods of synthesis of nanomaterials – hydrothermal synthesis, solvothermal synthesis – microwave irradiation– sol-gel and precipitation technologies – combustion flame – chemical vapour condensation process.

1.2 Gas-phase condensation synthesis – reverse micelle synthesis – polymer-mediated synthesis – protein microtubule-mediated synthesis – synthesis of nanomaterials using microorganisms and other biological agents – sonochemical synthesis – hydrodynamic cavitation.

1.3 Inorganic nanomaterials – typical examples – nano TiO_2/ZnO/CdO/CdS, organic nanomaterials – examples – rotaxanes and catenanes.

UNIT- II **15 Hours**

Characterisation of Nanoscale Materials

2.1. Principles of Atomic Force Microscopy (AFM) – Transmission Electron Microscopy (TEM).

2.2. Resolution and Scanning Transmission Electron Microscopy (STEM) – Scanning Tunnelling Microscopy (STM) – Scanning Nearfield Optical Microscopy (SNOM).

2.3. Scanning ion conductance microscope, scanning thermal microscope, scanning probe microscopes and surface plasmon spectroscopy.

UNIT- III **15 Hours**

Carbon Clusters and Nanostructures

3.1. Nature of carbon bond − new carbon structures − carbon clusters-carbon nanotubes – synthesis − single walled carbon nanotubes.

3.2. Structure and characterization − mechanism of formation − chemically modified carbon nanotubes − doping − functionalizing nanotubes − applications of carbon nanotubes.

3.3. Nanowires −synthetic strategies − gas phase and solution phase growth− growth control − properties.

UNIT- IV **15 Hours**

Nanotechnology and Nanodevices

4.1. DNA as a nanomaterial – DNA – knots and junctions, DNA – nanomechanical device designed by Seeman.

4.2. Force measurements in simple protein molecules and polymerase – DNA complexes– molecular recognition and DNA based sensor.

4.3. Protein nanoarray, nanopipettes, molecular diodes, self-assembled nanotransistors, nanoparticle mediated transfection.

UNIT- V **15 Hours**

Nanosensors & Biosensors

5.1. Nanosensors: introduction- characteristics and terminology – static and dynamic characteristics. Micro and nano-sensors, fundamentals of sensors, biosensor, micro fluids.

5.2. Packaging and characterization of sensors, sensors for aerospace and defense. Organic and inorganic nanosensors.

5.3. Biosensors: clinical diagnostics, generation of biosensors, nanomaterial based biosensors, biosensors based on nucleotides and DNA, electron transfer of biomolecules.

BOOKS FOR STUDY:

1. Patrick Solomon, *A Handbook on Nanochemistry*, 1st Ed., Dominant Publishers and Distributors, 2008.

2. Kenneth, J. Klabunde, *Nanoscale Materials in Chemistry*, 1st Ed., John Wiley and Sons Inc., Publications, 2009.

3. Mick Wilson, *Nanotechnology-Basic Science and Emerging Technologies*, 1st Ed., Overseas Press Private Ltd., 2008.

BOOKS FOR REFERENCE:

1. Rao, C. N. R., Muller, A. & Cheetham, A. K., *The Chemistry of Nanomaterials,* 1st Ed., Vol. 1 & 2; Wiley-VCH, Germany, Weinheim, 2004.
2. Pradeep, T., *Nano: The Essentials in Understanding Nanoscience and Nanotechnology,* 1st Ed., Tata McGraw Hill, New York, 2007.

WEB SOURCES:

1. Home page of Prof. Ned Seeman - http://seemanlab4.chem.nyu.edu/
2. Nanoletters - http://pubs.acs.org/journals/nalefd/index.html
3. Nanotation - http://www.acsnanotation.org/

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	summarize the synthetic methods of nanomaterials	K2
CO2	explain the various techniques of characterisation (AFM, SEM, TEM) for structural study of nanoscale materials	K3
CO3	compare and contrast various nano structures-nano clusters, nanotubes, nanowires	K3
CO4	discuss the application of nanotechnology in nanodevices	K6
CO5	examine the use of nanomaterials as organic and inorganic nanosensors and biosensors	K4

K2-Understand; K3-Apply; K4-Analyse; K6-Create

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	L	S	S	S
CO2	S	L	S	S	S
CO3	S	S	S	S	S
CO4	S	L	M	S	S
CO5	S	S	M	S	S

S- Strong; M- Medium; L- Low

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : EXTRA DISCIPLINARY COURSE: THERAPEUTICAL CHEMISTRY

COURSE CODE : 22PCHEDC HOURS/WEEK: 4 CREDIT: 4

SEMESTER : III

Course Objectives:

- *To know the terms of pharmacology.*
- *To learn about medicinal flora in India.*
- *To understand the common diseases and their cure.*
- *To acquire knowledge about antibiotics, sulpha drugs etc., & to understand the drugs used for diabetes, cancer and hypertension.*
- *To have general awareness on blood grouping, first aid, vitamins and hormones*.

SYLLABUS

UNIT-I 12 Hours

Introduction

1.1 Important terminologies used in medicinal chemistry – pharmacology, drug, pharmacognosy, pharmacy, therapeutics, toxicology, chemotherapy, pharmacopoeia, viruses, bacteria, vaccines, therapeutic index, encapsulation.

1.2 Routes of drug administration.

UNIT-II 12 Hours

Medicinal Flora in India:

2.1 Some Indian healers and their significance – neem, adathoda vasica, amla, turmeric, thulasi, thoothuvalai, kizhanelli, shoe flower.

2.2 Cancer curing plants.

2.3 Medicinal plants in the kitchen garden.

2.4 Spices as medicine.

2.5 Ayurveda and siddha medicines.

UNIT-III 12 Hours

Common diseases and Drugs (Reason and treatment)

3.1 Common air borne diseases – common cold, influenza, measles, mumps, diphtheria, whooping cough, tuberculosis.

3.2 Common water borne diseases – dysentery, cholera, typhoid, jaundice.

3.3 Common insect-borne diseases – malaria, elephantiasis.

3.4 Some other common diseases – asthma, epilepsy.

UNIT-IV **12 Hours**

Classification of Drugs

4.1 Sulpha drugs, antibiotics, analgesics, antiseptics and disinfectants, anaesthetics, psychopharmacology.

4.2 Life-style diseases and treatment- obesity, diabetes, cardiovascular diseases including blood pressure, cancer, AIDS. [Reason, drugs (Structure not needed), prevention].

UNIT-V **12 Hours**

Miscellaneous topics

5.1 Blood groups, Rh factor, composition of blood, types of anaemia and drugs.

5.2 Accidents and first aids.

5.3 Poisons and antidotes.

5.4 Vitamins and hormones.

5.5 Analysis of blood and urine.

BOOKS FOR STUDY:

1. Lakshmi, S., *Pharmaceutical Chemistry*, Sultan Chand & Sons, 3rd Ed., 2004.
2. Jayashree Ghosh., *Fundamental Concepts of Applied Chemistry*, 1st Ed., S. Chand, 2006.
3. Patrick, G.L., *An Introduction to Medicinal Chemistry*, 4th Ed., Oxford University Press, 2009.

BOOKS FOR REFERENCE:

1. Jayashree Ghosh., *A Text Book of Pharmaceutical Chemistry*, 3rd Ed., S. Chand, 2003.
2. Nogrady, T., & Weaver, D. F., *Medicinal Chemistry-A Molecular and Biochemical Approach*, Oxford University Press, 2005.

WEB SOURCES:

1. https://www.pharmapproach.com/routes-of-drug-administration/
2. https://www.drugs.com/drug-class/analgesics.html
3. https://academic.oup.com/bjaed/article/14/3/106/340726

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	relate the terminologies of therapeutical chemistry	K2
CO2	explain the different diseases and their treatment	K2
CO3	classify diseases and various types of drugs	K2
CO4	choose the appropriate medicinal herbs for healing	K3
CO5	justify the role of various factors on health and diseases	K5

K2-Understand; K3-Apply; K5-Evaluate

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : CORE-XIV: PHYSICAL METHODS IN CHEMISTRY

COURSE CODE : 22PCHC9 HOURS/WEEK: 6 CREDITS: 5

SEMESTER : IV

Course Objectives:

- *To study the principles and mechanism of PES and Mossbauer spectroscopy.*
- *To apply the different spectral techniques in understanding the structure of inorganic systems.*
- *To understand principles and applications of fluorescence and Laser spectroscopy.*

SYLLABUS

UNIT-I 18 Hours

Photoelectron spectroscopy and Mossbauer spectroscopy

1.1. Principle of PES, Koopman's theorem, PES spectra of HCl, HBr, HI, CO, NH_3, N_3^-, N_2, O_2, H_2O.

1.2. Photo electron spectroscopy in the study of bonding, anti-bonding and non-bonding orbitals, applications of PES.

1.3 Mossbauer spectroscopy: theory and principle of Mossbauer spectroscopy-Doppler effect, isomer shift, quadrupole interactions and magnetic interactions, applications to tin and iron compounds.

UNIT-II 18 Hours

Vibrational Spectra

2.1. Selection rules, mutual exclusion principle, application of IR and Raman to structural determination of inorganic compounds such as NSF_3, ClF_3, N_2O, SO_2, NO_3^-& ClO_3^-.

2.2 Site symmetry lowering-calcite and aragonite, identification of cis-trans isomers, linkage isomers, ionisation isomers, hydrate isomers.

2.3 Change in spectra of donor molecule upon coordination.

2.4. Use of group vibrations in the structural elucidation of complexes of urea, thiourea, cyanide, thiocyanate and DMSO.

2.5. IR spectra of carbonyls.

UNIT-III 18 Hours

NMR & EPR spectrosopy

3.1. Application of spin-spin coupling to structure determination.

3.2. ^{19}F NMR Spectra of ClF_3, $F_2PO(OH)$, $FPO(OH)_2$, BrF_5.

3.3. ^{31}P NMR Spectra of $HP_2O_5^{3-}$, HPF_2, $HPO(OH)_2$, P_4S_3 and $H_2PO(OH)$ ^{11}B NMR spectra of $B_3H_8^-$.

3.4. Theory, g value, factors affecting g, hyperfine splitting, fine splitting.

3.5. Zero field splitting and Kramer's degeneracy, EPR spectra of bissalicylaldimine Copper (II) complexes & $[Mn(H_2O)_6]^{2+}$. Applications of EPR.

UNIT –IV **18 Hours**

4.1. Phenomenon of fluorescence- -fluorescence spectroscopy-instrumentation,

4.2. Fluorophores-intrinsic or natural fluorophore-extrinsic fluorophores-DNA probes-chemical sensor probes-protein sensors-overview of effect of solvent on fluorescence.

4.3. Quenching of fluorescence-examples of some quenchers-oxygen as a quencher.

4.4. Applications of fluorescence spectroscopy-non-invasive monitoring of physiological parameters-mechanism of sensing-oxygen sensor-$[Ru(Ph_2phen)_3]^{2+}$.

4.5. Chloride sensor-pH and pCO_2 sensor-metal ion and anion sensor-glucose sensing by energy transfer.

UNIT-V **18 Hours**

5.1. Laser spectroscopy- Non-Linear Optical effects- frequency generation by Non-Linear Optical techniques-methods of obtaining population inversion.

5.2. Laser cavity modes, Q- switching, mode locking, sources for laser spectroscopy-solid state lasers- dye lasers, gas laser, semiconductor laser, Helium -Neon laser.

5.3. Laser profilometry-principle and its application in surface study.

5.4. Fluorescence excitation spectroscopy-laser induced fluorescence, laser magnetic resonance.

5.5. Photo acoustic spectroscopy, thermal lensing spectroscopy.

BOOKS FOR STUDY:

1. Ebsworth, E.A.V., Rankin, D.W.H., & Craddock, S., *Structural Methods in Inorganic Chemistry*, 1st Ed., ELBS, 1987.

2. Veera Reddy K., *Symmetry and Spectroscopy of Molecules*, 2nd Ed., New Age International Ltd., 2009.

3. Drago, R.S., *Physical Methods in Chemistry*, Reinhold, Saunders College Publishing, USA, 1977.

4. Joseph, R., Lakowicz., *Principles of Fluorescence Spectroscopy*, 3rd Ed., Springer, 2006**.**

5. Aruldhas, G., *Molecular Structure and Spectroscopy*, 2nd Ed., Eastern Economy Edition, 2007.

BOOKS FOR REFERENCE:

1. Gurdeep, R. Chatwal & Sham, K. Anand, *Instrumental Methods of Chemical Analysis*, 5th Ed., Himalaya Publishing House, Mumbai, 2007.

2. Michael Hollas J., *Modern Spectroscopy*, 4th Ed., Wiley India Edition, 2010.

WEB SOURCES:

1. https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Spectroscopy/Magnetic_Resonance_Spectroscopies/Electron_Paramagnetic_Resonance/EPR_-_Interpretation

2. https://nptel.ac.in/content/syllabus_pdf/104104084.pdf

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	demonstrate the basic concepts underlying PES, MB, fluorescence, laser, NMR, IR and EPR spectroscopy with reference to inorganic compounds	K2
CO2	examine the effect of hyperfine and fine splitting in EPR spectroscopy and quadrupolar splitting in MB spectroscopy	K4
CO3	compare the spin-spin coupling in hetero nuclear NMR spectroscopy	K2
CO4	solve the structure of inorganic molecules by applying IR, NMR, EPR and MB spectroscopy	K6
CO5	apply the fluorescence spectroscopy for sensors.	K3

K2-Understand; K3-Apply; K4-Analyse; K6-Create

Mapping of COs with POs

COs	POs				
	PO1	**PO2**	**PO3**	**PO4**	**PO5**
CO1	S	S	S	S	S
CO2	S	S	S	S	S
CO3	S	S	S	S	S
CO4	S	S	S	S	S
CO5	S	M	M	S	S

S- Strong; M- Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : ELECTIVE – IV: INTRODUCTION TO CHEMINFORMATICS AND COMPUTER AIDED DRUG DESIGN

COURSE CODE : 22PCHEC4 HOURS/WEEK: 6 CREDITS: 5

SEMESTER : IV

Course Objectives:

- *To understand the concepts of cheminformatics.*
- *To have the basic idea QSAR in drug designing.*
- *To have a hands on skills on various softwares used in drug designing.*
- *To have an overview on molecular modelling methods.*

SYLLABUS

UNIT-I **18 Hours**

Introduction to Cheminformatics

1.1 History and evolution of cheminformatics, use and prospects of cheminformatics.

1.2 Computer representations of chemical structures-graph theoretic representations of chemical structures-connection tables, SMILES notation-writing smiles for small molecules (ethane, benzene, cyclohexane, 2-methyl propane, cis and trans butene, succinic acid and acetic acid)-

1.3 Canonical representations of molecular structures, databases and searches- structure, reaction, patent and relational data bases. 3D DATABASES-Cambridge Structural Database (CSD), Protein Data Bank (PDB)- 3D Pharmacophores.

UNIT-II **18 Hours**

Quantitative Structure Activity Relationship

2.1 QSAR descriptors calculated from the 2D structure-simple counts-hydrogen bond donors, hydrogen bond acceptors, ring systems (including aromatic rings), rotatable bonds and molecular weight.

2.2 Physicochemical properties – hydrophobicity - partition coefficient-substituent hydrophobicity constant – effect of log p on drugs- a case study of a cardiotonic drug.

2.3 Electronic effects-its role in insecticidal activity of drugs, steric factors-Taft steric factor- molar refractivity. Isosteres, identification of a pharmacophore.

UNIT-III **18 Hours**

Towards Drug Designing

3.1 Virtual screening-need and uses; "drug-likeness" and compound filters- Lipinski rule of 5, ADMET properties-hydrogen bonding descriptors, polar surface area, toxicity prediction.

3.2 Drug optimizations and strategies in drug design: variation of substituents, extension of structure, chain extension or contraction, ring expansion /contraction, ring variations, ring fusions.

3.3 Drug design by NMR - docking- a preliminary idea, automatic docking, manual docking, rigid docking.

UNIT-IV **18 Hours**

Molecular Modelling Methods

4.1 Molecular and quantum mechanics methods for electronic structure study- an overview.

4.2 Drawing chemical structure using chemdraw and exploring its features, chem 3D, Rasmol etc.

4.3 Study of molecular properties—partial charges, molecular electrostatic potential, Molecular orbitals, spectroscopic charges-structure comparison and overlays using chem 3D. Using ZINC data base for drug searching.

UNIT-V **18 Hours**

Softwares and their Application in Drug Designing

5.1 Calculation of molecular properties and bioactivity score using Molinspiration-hands on training on many molecules.

5.2 CRDD web portal-computational resources for drug discovery- a thorough surfing of the web page-familiarity with freely available databases listed there-using PK tutor.

5.3 OSIRIS property explorer, data warrior-toxicity, Log P, drug-likeness prediction, Swiss ADME – drug-likeness prediction-parameters-bioavailability radar- synthetic accessibility and lead-likeness of various molecules.

BOOKS FOR STUDY:

1. Leach, A. R., & Valerie, G., *An introduction to Chemoinformatics,* Springer, 2007.
2. Patrick, G. L., *An Introduction to Medicinal Chemistry*, 4th Ed., Oxford University Press, 2009.

3. Roy, K., Kar, S., & Das, R. N., *A Primer on QSAR/QSPR Modelling Fundamental Concepts*, Springer Cham Heidelberg, 2015.
4. Cramer, C.J., *Essentials of Computational Chemistry: Theories and Models*, John Wiley & Sons, 2004.

BOOKS FOR REFERENCE:

1. Leszczynski, J., Kedziera, A, K., Puzyn, T., Papadopoulos, M.G., Reis, H., & Shukla, M.K., *Handbook of Computational Chemistry*, 2nd Ed., Springer International Publishing, 2017.
2. Fujita, T., *QSAR and Drug Design: New Developments and Applications*, Elsevier, 1995.
3. Kubinyi, H., *QSAR: Hansch Analysis and Related Approaches*, Weinheim- VCH, 1993.
4. Bachrach, S.M., *Computational Organic Chemistry*, John Wiley & Sons, Inc. 2007.

WEB SOURCES:

1. https://nptel.ac.in/courses/102/106/102106070/
2. http://zinc.docking.org/substances/home/
3. https://www.molinspiration.com/cgi-bin/properties
4. http://crdd.osdd.net/
5. https://www.organic-chemistry.org/prog/peo/
6. http://www.swissadme.ch/index.php
7. http://media.cambridgesoft.com/support/manuals/16/ChemDrawHelp.pdf
8. http://www.openrasmol.org/doc/rasmol.html

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	apply the basic concepts of cheminformatics	K3
CO2	evaluate the role of QSAR in drug designing	K5
CO3	infer the importance of virtual screening and docking	K2
CO4	explain different molecular modelling techniques	K2
CO5	apply various softwares like Molinspiration, Swiss ADME, ZINC, OSIRIS in elementary analysis of drug design	K3

K2-Understand; K3-Apply; K5-Evaluate

Mapping of COs with POs

COs	POs				
	PO1	**PO2**	**PO3**	**PO4**	**PO5**
CO1	S	S	S	S	S
CO2	S	S	S	S	S
CO3	S	S	S	S	S
CO4	S	M	S	S	S
CO5	S	S	S	S	S

S- Strong; M- Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : ELECTIVE-IV: SOLID STATE CHEMISTRY

COURSE CODE : 22PCHESC4 HOURS/WEEK: 6 CREDITS: 5

SEMESTER : IV

Course Objectives:

- *To learn the crystal structures of few inorganic solids.*
- *To study the chemistry of crystallization and vapour phase transport.*
- *To learn the applications of magnetic materials.*
- *To study the chemistry of organic solids.*

SYLLABUS

UNIT I **18 Hours**

Crystal Structure and Crystal Engineering of Organic Solids

1.1. Types of close packing – HCP and CCP – packing efficiency – SC, BCC, and FCC, radius ratio rule – applications – polyhedral description of solids – structure types: Na_2O, Cs_2O, ReO_3, K_2NiF_4.

1.2. Hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs – concepts of different types of synthons based on non-covalent interactions – principles of crystal engineering and non-covalent synthesis.

1.3. Polymorphism and pseudo - polymorphism – supramolecular isomorphism, polymorphism and crystal engineering of pharmaceutical phases.

UNIT II **18 Hours**

Preparative Methods in Solid State Chemistry

2.1. Experimental procedure, co-precipitation as a precursor to solid state reaction, other precursor methods, kinetics of solid state reactions – crystallizations of solutions, melts, glasses and gels, solutions and gels.

2.2. Zeolite synthesis – precipitation from solution or melt: flux method, epitaxial growth of thin layers, verneuil flame fusion method. Graphite intercalation compounds, transition metal dichalcogenide and other intercalation compounds, ion exchange reaction, synthesis of new metastable phases by ‘Chimie Douce’.

2.3. Electrochemical reduction methods – preparation of thin films, chemical and electrochemical methods, physical methods – growth of single crystals, Czochralski method, Bridgman-Stockbarger methods – zone melting. Vapour phase transport, hydrothermal methods, comparison of different methods – high pressure and hydrothermal methods and dry high pressure methods.

UNIT III **18 Hours**

Metallo Organic Frameworks

3.1. Metallo Organic Frameworks (M.O.Fs) – organometallic systems – combinations of different interactions to design molecular rods, triangles, ladders, networks, etc.

3.2. Design of nanoporous solids. Inter-ligand hydrogen bonds in metal complexes.

3.3 Implications for drug design – crystal engineering of NLO and OLED materials.

UNIT IV **18 Hours**

Magnetic Materials and Optical Properties

4.1. Selected examples of magnetic materials and their properties – metals and alloys, transition metal oxides, spinels, garnets, ilmenite and perovskites.

4.2. Magnetoplumbites – applications – structure/property relations – transformer, information storage, magnetic bubble memory devices, permanent magnets.

4.3. Luminescence, Lasers and phosphors – definitions and general comments, configurational coordinate model, some phosphor materials, anti-Stokes phosphors – lasers – the ruby laser, neodymium lasers.

UNIT V **18 Hours**

Organic Solid State Chemistry

5.1. Topochemical control of solid state organic reactions – intramolecular reactions – conformational effects – intermolecular reactions – molecular packing effects – photodimerization of 2-ethoxycinnamic acid (α, β, γ forms) – photopolymerization of 2,5-distyrylpyrazine – photopolymerizations of diacetylenes.

5.2. Asymmetric syntheses – dimerization of anthracene – control of molecular packing arrangements.

5.3. Organic reactions within inorganic host structures – electrically conductive organic solids – organic metals, conjugated systems, doped polyacetylene, polyparaphenylene, polypyrrole – organic charge transfer complexes – new superconductors.

BOOKS FOR STUDY:

1. West, A. R., Solid *State Chemistry and its Applications*, 2nd Ed., John Wiley and Sons, New York, 2014.
2. Lehn, J. M., *Supramolecular Chemistry*, 1st Ed., Wiley, 1995.

BOOKS FOR REFERENCE:

1. Moore, E. A., Smart, L. E., *Solid State Chemistry*, 5th Ed., CRC Press, 2021.
2. Woodward P, Vogt, T, John Evans, S. O. Karen P., *Solid State Materials Chemistry*, 1st Ed., Cambridge University Press, 2021.

WEB SOURCES:

1. Crystal Growth and Design. http://www.pubs.acs.org/journals/ cgdefu/index.html
2. Crystal Engineering Communication, http://www.rsc.org /Publishing/ Journals /ce/ index.asp

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	classify the crystal structure and explain the principles of crystal engineering and non-covalent synthesis	K2
CO2	determine the structure and coordination number of ionic solids	K5
CO3	explain various preparatory methods for organometallic solids and their applications	K2
CO4	relate the magnetic materials and their optoelectric property	K3
CO5	outline the aspects of solid state organic polymers	K2

K2-Understand; K3-Apply; K5-Evaluate

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	L	S	S	S
CO2	S	L	S	S	S
CO3	S	L	S	S	S
CO4	S	M	S	S	S
CO5	S	M	S	S	S

S- Strong; M- Medium; L- Low

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : ELECTIVE V: ORGANIC PHOTOCHEMISTRY AND SPECTROSCOPY

COURSE CODE : 22PCHEC5 HOURS/WEEK: 6 CREDITS: 5

SEMESTER : IV

Course Objectives:

- *To understand the principles of organic photochemistry.*
- *To gain knowledge about pericyclic reactions, cycloaddition and sigmatropic rearrangements.*
- *To apply the spectral techniques in the structural elucidation of organic compounds.*

SYLLABUS

UNIT- I **18 Hours**

Organic Photochemistry

1.1 Introductory theory of light absorption, photophysical processes- Jablonski diagram, IC, ISC, fluorescence and phosphorescence.

1.2 Photochemical reactions of ketones – Norrish type I and II, Paterno-Buchi reaction, Photoreduction of ketones, photo induced reactions of α, β -unsaturated ketones,

1.3 Photochemistry of alkenes – photodimerization, cis-trans isomerisation and photosensitization of butadiene, photochemical oxidation.

UNIT- II **18 Hours**

Pericyclic Reactions, Cycloadditions and Sigmatropic Rearrangements

2.1 Pericyclic reactions - molecular orbital symmetry, frontier orbitals of ethylene, 1, 3-butadiene, 1, 3, 5- hexatriene- classification of pericyclic reactions- electrocyclic reactions – 4n and 4n+2 systems, Woodward –Hoffmann rules, correlation diagram, FMO and PMO approach [1, 3-dienes and 1, 3, 5-trienes] .

2.2 Cycloadditions - antarafacial and suprafacial additions, 4n and 4n+2 systems, 1, 3-dipolar addition, Diel's-Alder reaction.

2.3 Sigmatropic rearrangements - suprafacial and antarafacial shifts of hydrogen, Cope, Claisen and di-π methane rearrangements.

UNIT- III **18 Hours**

UV-Visible and IR Spectroscopy

3.1 UV-Visible spectroscopy – principle, types of excitation, transition probabilities-chromophores and auxochromes-factors affecting intensity-solvent effect and position of absorption bands-dienes, polyenes and enones.

3.2 IR Spectroscopy – principle, characteristic group frequencies of organic molecules-factors influencing vibrational frequencies, interpretation of IR spectra of organic molecules.

3.3 UV-Visible spectroscopy - Woodward- Fieser rule, applications of UV spectroscopy, IR spectroscopy - application of IR spectroscopy – hydrogen bonding, distinction between cis-trans isomers.

UNIT- IV **18 Hours**

NMR spectroscopy

4.1 Proton nmr- Principle -chemical shift, factors affecting chemical shift-number of signals-peak areas-multiplicity-geminal, vicinal and long range coupling-factors affecting them-first order spectra.

4.2 Simplification technique -chemical and instrumental techniques, applications of NMR spectroscopy.

4.3 ^{13}C NMR-broad band and off- resonance -decoupling-comparison of ^{1}H and ^{13}C NMR-factors affecting intensity of signals-chemical shifts-γ gauche effect. Elementary idea of 2D NMR - COSY, NOSY, ROSY.

UNIT-V **18 Hours**

Mass Spectrometry and Structural Elucidation

5.1 Mass spectrometry - basic principle-molecular ion peak, parent ion peak, fragments, meta stable ion peaks, isotope peaks -determination of molecular weight and molecular formula–McLafferty rearrangement-rules for fragmentation-nitrogen rule, ring rule.

5.2 Examples of mass spectral fragmentation of organic compounds – alkanes, alkenes, aromatic hydrocarbons, alkyl halides, aldehyde, ketones, alcohols, phenols, acids, esters and amines.

5.3 Structural elucidation - structural elucidation of organic compounds using the combination of UV, IR, NMR and mass spectral techniques (molecular formula of organic compound restricted to 12 carbons).

BOOKS FOR STUDY:

1. Biswanath Dinda, *Essentials of Pericyclic and Photochemical Reactions,* 1st Ed., Springer, 2017.
2. Paula Yurkanis Bruice, *Organic Chemistry,* 8th Ed., Pearson Education, 2015.
3. Carey, F.A., & Sundberg, R.J., *Advanced Organic Chemistry,* Part A Springer, 2007.
4. Jag Mohan, *Organic Spectroscopy – Principles and Applications,* 2nd Edition, Narosa Publishing House, New Delhi, 2009.
5. Sharma, Y. R., *Elementary Organic Spectroscopy,* Revised Ed., S. Chand & Company Ltd. New Delhi, 2013.

BOOKS FOR REFERENCE:

1. Mukherjee, K.S., *Mechanism of Organic Reactions*, 1st Ed., Books and Allied (p) Ltd 2012.
2. Kemp, G. W., *Organic Spectrscopy*, 3rd Ed., Mc Millan Ltd. 2019.
3. Silverstein, R.M. Bassler, G.C., Morrill, T.C., *Spectrometric Identification of Organic Compounds,* 2th Ed., John Wiley & Sons, 1991.

WEB SOURCES:

1. https://www.med.unc.edu/microscopy/files/2018/06/jablonski-diagram.pdf
2. https://www.masterorganicchemistry.com/2016/11/29/ir-spectroscopy-some-simple-practice- problems/
3. https://www.masterorganicchemistry.com/2016/09/27/uv-vis-spectroscopy-some-practice-questions/
4. https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Spectroscopy/Magnetic_Resonance_Spectroscopies/Nuclear_Magnetic_Resonance/NMR%3A_Structural_Assignment/NMR14._More_Practice_with_NMR_Spectroscopy
5. https://chem.libretexts.org/Courses/Purdue/Purdue%3A_Chem_26200%3A_Organic_Chemistry_II_(Wenthold)/Chapter_11%3A__IR_and_Mass_Spectrometry/11.09_Solving_Problems_using_Mass_Spectrometry

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	categorize the role of photochemistry and its applications in organic synthesis	K4
CO2	predict the products on pericyclic reactions	K4
CO3	apply the theories of UV, IR, NMR and mass spectral techniques for structural elucidation	K3
CO4	explain the factors affecting and applications of UV, IR, NMR and mass spectra	K5
CO5	interpret the UV, IR, NMR and mass spectral data and deduce the structure of organic compounds	K5

K3-Apply; K4-Analyse; K5-Evaluate

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	L	S	S	S
CO2	S	L	S	S	S
CO3	S	S	S	S	S
CO4	S	S	S	S	S
CO5	S	S	S	S	S

S-Strong; L- Low

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : ELECTIVE-V: MEDICINAL CHEMISTRY

COURSE CODE : 22PCHESC5 HOURS/WEEK: 6 CREDIT: 5

SEMESTER : IV

Course Objectives:

- *To gain knowledge about analgesics and anaesthetics.*
- *To know about anti-histamine and anti-inflammatory drugs.*
- *To understand about expectorants and antitussives.*

SYLLABUS

UNIT- I **18 Hours**

Basic concepts

1.1 Drug design- factors governing drug design, method of variation and tailoring of drugs; physical properties- factors governing drug action at active site, factors governing ability of drugs to reach active site.

1.2 General anaesthetics-inhalation anaesthetics, intravenous anaesthetics and basal anaesthetics- mode of action, local anaesthetics- classification.

1.3 Sedatives and hypnotics- classification and synthesis, mode of action.

UNIT – II **18 Hours**

Anticonvulsants, stimulants and anti-pyretic analgesics

2.1 Anti-convulsants- classification, synthesis and mode of action. Muscle relaxants- classification, synthesis and mode of action.

2.2 Central nervous system- stimulants- classification, synthesis and mode of action.

2.3 Antipyretic analgesics- classification, synthesis and mode of action.

UNIT – III **18 Hours**

Other analgesics

3.1 Narcotic or opiate analgesics- classification, synthesis and mode of action; narcotic antagonist.

3.2 Cardiovascular drugs- classification, cholinomimetic drugs- antimuscarinic drugs, ganglionic blocking agents and adrenegic neuron blocking agents.

3.3 Diuretics- synthesis and mode of action of mercurial and non-mercurail diuretics.

UNIT – IV **18 Hours**

Anti-histamines and anti-inflammatory drugs

4.1 Anti-histaminics- synthesis and mode of action of histamine H_1 receptor antagonists and histamine H_2 receptor blockers-prevention of histamine release; structure- activity relationship amongst H_1 receptor blockers.

4.2 Non-steroidal anti-inflammatory drugs (NSAID) - synthesis and mode of action of heteroaryl acetic acid analogues, aryl acetic acid analouges.

4.3 Aryl propionic acid analogues, naphthalene acetic acid analogues, gold compounds, salicyclic acid analogues, pyrazolones and pyrazolodiones.

UNIT – V **18 Hours**

Expectorants and Antitussives

5.1 Synthesis and mode of action of sedative expectorants, stimulants expectorants and centrally active antitussive agents- sulphonamides- synthesis and mode of action of sulphonamides.

5.2 Antimalarials- synthesis and mode of action of aminoquinoline analogues, aminoacridine analoges, guanidine analogues, pyrimidine analogues, sulphone and quinine analogues- cardiac glycosides, bile acids.

5.3 Antibiotics- synthesis and mode of action of penicillins, amino glycoside antibiotics, chloramphenicol and tetracyclines.

BOOKS FOR STUDY:

1. Lakshmi, S., *Pharmaceutical Chemistry*, 3rd Ed., Sultan Chand & Sons, 2004.
2. Jayashree Ghosh., *Fundamental concepts of Applied Chemistry*, 1st Ed., Sultan Chand & Sons, 2006.
3. Patrick, G. L., *An Introduction to Medicinal Chemistry*, 4th Ed., Oxford University Press, 2009.

BOOKS FOR REFERENCE:

1. Jayashree Ghosh., *A Text Book of Pharmaceutical Chemistry,* 3rd Ed., S.Chand, 2003.
2. Nogrady, T., & Weaver, D. F., *Medicinal Chemistry- A Molecular and Biochemical Approach*, Oxford University Press, 2005.
3. Ashutosh Kar, *Medicinal Chemistry*, 3rd Ed., New Age International (P) Ltd., New Delhi, 2005.

WEB SOURCES:

1. https://www.drugs.com/drug-class/analgesics.html

2. https://academic.oup.com/bjaed/article/14/3/106/340726

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	explain the basic concepts about drugs	K2
CO2	classify various drugs and illustrate their synthesis	K3
CO3	compare the mode of actions of different drugs	K4
CO4	identify suitable drugs for diseases	K4
CO5	develop ideas on drug design	K3

K2-Understand; K3-Apply; K4-Analyse

Mapping of COs with POs

COs	POs				
	PO1	**PO2**	**PO3**	**PO4**	**PO5**
CO1	S	M	S	S	S
CO2	S	M	S	S	S
CO3	S	M	S	S	S
CO4	S	S	S	S	S
CO5	S	M	S	S	S

S-Strong; M- Medium

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : ORGANIC CHEMISTRY PRACTICAL-II

COURSE CODE : 22PCHQC4 HOURS/WEEK: 3+3 CREDITS: 3

SEMESTER : III & IV

Course Objectives:

- *To develop the skills of separation and identification of organic compounds.*
- *To enlighten the students in the analysis of spectra of simple organic compounds.*

SYLLABUS

1. Organic analysis- separation of two & three component mixtures-identification of components and preparation of their derivatives.
2. Recording the IR Spectra and interpretation of an aldehyde, a ketone, an alcohol, a phenol and an amine.
3. Recording the Fluorescence spectra and its interpretation for any two carbonyl compounds.
4. Solving Combo problems by using UV, IR, ^{1}H, ^{13}C NMR and Mass spectral data to identify the compounds such as aldehyde, ketone, alcohol, phenol and amine.

BOOKS FOR REFERENCE:

1. Gnanaprakasam, V.S., Ramamurthy, G., *Organic Chemistry Lab Manual*, Viswanathan Reprint Printers and Publishers Private Ltd. 2000.
2. Pavia, D. L., Lampman, G. M., Kris, G. S., Engel, R. G., *A Microscale Approach to Organic Laboratory Techniques*, 6th Ed., Cengage Learning, 2016.
3. Zubrick., J. W., *The Organic Chemistry Lab Survival Manual- A Student's Guide to Techniques*, 9th Ed., John Wiley & Sons, 2014.
4. Vishnoi, N.K., *Advanced Practical Organic Chemistry*, 2nd Reprint Hindustan Offset Printers, Delhi, 1994.
5. Sathish Agarwala & Agarwala, R. C., *Advanced Organic Analysis*, 2nd Revised Edition. Pragati Prakashan, Meerut, 1996.

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	categorize organic mixture by solvent extraction methods	K4
CO2	analyse the functional groups in an unknown organic mixture	K4
CO3	synthesize suitable derivatives for the organic compounds	K6
CO4	determine the functional group in organic compounds using IR spectrometer	K5
CO5	deduce the structure of organic compounds from the given spectral data	K5

K4-Analyse; K5-Evaluate; K6-Create

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	S	S	S	S
CO2	S	S	S	S	S
CO3	S	S	S	S	S
CO4	S	S	S	S	S
CO5	S	S	S	S	S

S- Strong

PROGRAMME TITLE : M.Sc. CHEMISTRY

COURSE TITLE : PHYSICAL CHEMISTRY PRACTICAL -II

COURSE CODE : 22PCHQC5 HOURS/WEEK: 3+3 CREDITS: 3

SEMESTER : III & IV

Course Objectives:

- *To study the mechanism of the reactions through kinetics.*
- *To introduce the concepts of estimations by conductivity measurements.*
- *To acquire the knowledge in using softwares for molecular modelling.*

SYLLABUS

1) Kinetic studies –acid hydrolysis of methyl acetate, $S_2O_8^{2-}$ +I^- reaction.
2) Conductivity –kinetics of the alkaline hydrolysis of ethyl acetate.
3) Salt effect on reaction rates, $S_2O_8^{2-}$ + I^- reaction.
4) Determination of activation energy, acid hydrolysis of methyl acetate .
5) Determination of order of reaction, $S_2O_8^{2-}$ + I^- reaction.
6) Conductometric titrations
    a) strong acid Vs strong base.
    b) strong acid Vs weak base.
    c) weak acid Vs strong base.
    d) Mixture of acids Vs strong base.
    e) KCl Vs $AgNO_3$.
    f) $BaCl_2$Vs K_2SO_4
7) Determination of K_a of strong electrolyte.
8) Determination of K_a of weak electrolyte.
9) Study the specific rotation of glucose using polarimeter.
10) Determination of association of ethyl acetate by sodium hydroxide conductomertically and determine the order of the reaction.
11) Compare the relative strength of acetic acid and monochloroacetic acid by conductivity method.
12) Determination of the optimized energy, IR and Raman frequencies and its graphical representation, NMR chemical shift and its graphical representation and HOMO-LUMO energy gap of some compounds with quantum chemistry computation software package Gaussian 09.

BOOKS FOR REFERENCE:

1. Viswanathan, B., & Raghavan, P. S., *Practical Physical Chemistry*, Viva Books Pvt. Ltd. 2005.
2. Levitt, B. P., *Findlay's Practical Physical Chemistry*, 9th Ed., Longman Group Ltd, 1988.
3. Yadav, J. B., *Advanced Practical Physical Chemistry*, 27th Ed., Goel Publishing House, 2008.

WEB SOURCES:

1. www.arguslab.com
2. www.Gaussian.com

Course Outcomes

On completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level
CO1	evaluate the relative strength of acids and energy of activation by kinetics	K5
CO2	examine the behaviour of strong and weak electrolytes	K4
CO3	identify the order of reaction	K3
CO4	develop skills in the estimation of acid-base and halides by conductometric methods	K3
CO5	use softwares for molecular modelling	K3

K3-Apply; K4-Analyse; K5-Evaluate

Mapping of COs with POs

COs	POs				
	PO1	PO2	PO3	PO4	PO5
CO1	S	S	S	S	S
CO2	S	S	S	S	S
CO3	S	S	M	S	S
CO4	S	S	S	S	S
CO5	S	S	M	S	S

S- Strong; M- Medium