



गोंय विद्यापीठ

ताळगांव पठार

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(Accredited by NAAC)

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GU/Acad –PG/BoS -NEP/2023/78/4

Date:24.05.2023

Ref: GU/Acad –PG/BoS -NEP/2022/339/11 dated 19.08.22

### CIRCULAR

In supersession to the above referred Circular, the updated approved Syllabus with revised Course Codes of the **Master of Science in Chemistry Programme** is enclosed.

The approved Syllabus of the **Master of Science in Chemistry** Programme (Organic, Inorganic, Analytical and Physical, Pharmaceutical Chemistry) is attached.

The Dean/ Vice-Deans of the School of Chemical Sciences/ Principals of Affiliated Colleges offering the **Master of Science in Chemistry** Programme are requested to take note of the above and bring the contents of the Circular to the notice of all concerned.

ASHWIN VYAS  
LAWANDE  
Date: 2023.05.24  
17:31:44 +05'30'

(Ashwin Lawande)

Assistant Registrar – Academic-PG

To,

1. The Dean, School of Chemical Sciences, Goa University.
2. The Vice-Deans, School of Chemical Sciences, Goa University.
3. The Principals of Affiliated Colleges offering the Master in Sciences in Chemistry Programme.

Copy to:

1. The Chairperson, Board of Studies in Chemistry PG.
2. The Programme Director, M. Sc. Chemistry, Goa University.
3. The Controller of Examinations, Goa University.
4. The Assistant Registrar, PG Examinations, Goa University.
5. Directorate of Internal Quality Assurance, Goa University for uploading the Syllabus on the University website.

**ANNEXURE-I****M.Sc. Chemistry (SEM I & II) Syllabus (80 Credit course) as per NEP 2020 for AY 2022-23**

<b>SEM I</b>			
<b>Sr. No.</b>	<b>Subject code</b>	<b>Paper title</b>	<b>Credits</b>
1.	<a href="#"><u>CHO-500</u></a>	Fundamentals of Organic Chemistry	4
2.	<a href="#"><u>CHI-500</u></a>	Fundamentals of Inorganic Chemistry	4
3.	<a href="#"><u>CHP-500</u></a>	General Physical Chemistry	4
4.	<a href="#"><u>CHA-500</u></a>	Techniques in Analytical Chemistry-I	4
5.	<a href="#"><u>CHO-521</u></a>	Practical Course in Organic Chemistry-I	2
6.	<a href="#"><u>CHO-522</u></a>	Practical Course in Organic Chemistry-II	2
7.	<a href="#"><u>CHI-521</u></a>	Practical Course in Inorganic Chemistry-I	2
8.	<a href="#"><u>CHI-522</u></a>	Practical Course in Inorganic Chemistry-II	2
9.	<a href="#"><u>CHP-521</u></a>	Practical Course in Physical Chemistry-I	2
10.	<a href="#"><u>CHP-522</u></a>	Practical Course in Physical Chemistry-II	2
11.	<a href="#"><u>CHA-521</u></a>	Practical Course in Analytical Chemistry-I	2
12.	<a href="#"><u>CHA-522</u></a>	Practical Course in Analytical Chemistry-II	2
<b>SEM II (Inorganic Chemistry)</b>			
1.	<a href="#"><u>CHI-501</u></a>	Chemistry of Coordination & Organometallic Compounds	4
2.	<a href="#"><u>CHI-502</u></a>	Chemistry of Materials	4
3.	<a href="#"><u>CHI-503</u></a>	Concepts in Molecular Symmetry and Spectroscopy	4
4.	<a href="#"><u>CHI-504</u></a>	Concepts in Inorganic Chemistry	4

<b>SEM II (Analytical Chemistry)</b>			
1.	<a href="#"><u>CHA-501</u></a>	Chemical Methods of Analysis	4
2.	<a href="#"><u>CHA-502</u></a>	Techniques in Analytical Chemistry-II	4
3.	<a href="#"><u>CHA-503</u></a>	Separation Techniques	4
4.	<a href="#"><u>CHA-504</u></a>	Instrumental Methods of Analysis	4
<b>SEM II (Organic Chemistry)</b>			
1.	<a href="#"><u>CHO-501</u></a>	Organic Spectroscopy	4
2.	<a href="#"><u>CHO-502</u></a>	Pericyclic and Organic Photochemical Reactions	4
3.	<a href="#"><u>CHO-503</u></a>	Synthetic Methodologies in Organic Chemistry	4
4.	<a href="#"><u>CHO-504</u></a>	Stereochemistry and Organic Transformations	4
<b>SEM II (Physical Chemistry)</b>			
1.	<a href="#"><u>CHP-501</u></a>	Quantum Chemistry and Statistical Thermodynamics	4
2.	<a href="#"><u>CHP-502</u></a>	Group Theory and Molecular Spectroscopy	4
3.	<a href="#"><u>CHP-503</u></a>	Chemical Kinetics and Thermodynamics	4
4.	<a href="#"><u>CHP-504</u></a>	Electrochemistry and Surface Studies	4

Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHA-500 Title of the course: Techniques in Analytical Chemistry - I

Number of Credits: 04

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied chemistry courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
<b>Course Objective:</b>	1. Learning various methods of data handling in analysis. 2. Understanding the significance of sampling and calibration techniques. 3. Understanding principles and applications of various types of techniques 4. Training the students to deduce structures based on IR, NMR, MS combined data.	
<b>Content:</b>	<b>1. Analytical Objectives and Data Handling</b> Importance of analytical chemistry in research and industry; statistics and data handling in analytical chemistry, standard operating procedures, good laboratory practices: quality assurance, method validation and quality control.	No. of Hours 5
	<b>2. Sampling and Calibration Techniques</b> Sampling and sample preparation, general steps in chemical analysis, calibration of glass wares. Finding the best straight line-least square regression, correlation coefficient; Calibration curves, standard addition technique and internal standards. Chemical concentrations.	5
	<b>3. Classical methods of Analysis</b> Gravimetry and Titrimetric methods, Principle, methodology, Advantages & Disadvantages over instrumental methods. Conditions for identifying a given reaction as method of Analysis, Classification of reactions in titrimetric analysis (Acid-Base, redox, complexometric and precipitation), Standard solutions and their preparation. Selection of Visual Indicators in titrimetric Analysis	6
	<b>4. Introduction to Electroanalytical techniques</b> Introduction to electrochemical cell, electrode potential, Classification of electroanalytical techniques, working principles, and their applications	4
	<b>5. Introduction to Thermoanalytical techniques</b> Principle, Instrumentation and applications of Thermo Gravimetric Analysis, Differential Thermal Analysis, and Differential Scanning Calorimetry. Numericals based on TGA.	5
	<b>6. Introduction to Chromatographic Techniques</b> a. Principles of chromatography, classification of	15

	<p>chromatographic techniques based on mechanism of retention, configuration, mobile and stationary phase. Efficiency of separation- plate theory (theoretical plate concept) and rate theory (van Deemter equation).</p> <p>b. Principles and applications of Paper chromatography, thin layer chromatography, HPTLC, Size exclusion and Ion exchange chromatography. Counter-current chromatography for isolation of natural products.</p> <p>c. Gas and Liquid Chromatography: Introduction; Instrumental Modules; The Separation System; Choice of Conditions of Analysis; Sample Inlet Systems; Detectors; Practical Considerations in Qualitative and Quantitative Analysis; Coupled Systems-introduction to GCMS, LCMS; Applicability-interpretation and numericals.</p>	
	<p><b>7. Introduction to Spectroscopic Techniques</b></p> <p>a. Interaction of Electromagnetic Radiation with Matter: Electromagnetic spectra, regions of spectrum, numericals.</p> <p>b. Ultraviolet and visible Spectroscopy: Electronic spectra and Molecular structure: types of electronic transition, Chromophore and auxochrome, absorption by isolated chromophore, conjugated chromophores, aromatic compounds, inorganic chelates. Calculating <math>\lambda_{max}</math> for Conjugated Dienes, Trienes, polyenes, <math>\alpha,\beta</math>-unsaturated carbonyl compounds, Numericals. Choices and effect of solvents on UV-Vis. Quantitative Calculations: Beer-Lambert Law; Mixtures of absorbing species-laws of additivity of absorbance; calibration curve for calculation of unknown; Spectrometric errors in measurement; Deviation from Beer-Lambert Law - chemical deviation, instrumental deviation; Numericals for quantitative analysis using UV-VIS spectroscopy.</p> <p>c. Infrared Spectroscopy: Infrared absorption and molecular structures, molecular vibrations, types of vibrations, IR spectra, overtones and bands-basis of NIR absorption. Spectra interpretation, Frequencies of functional group, Spectral Databases, Identification of unknown compounds.</p> <p>d. Spectrometric Instrumentation of UV-Vis and IR: Sources, monochromators, sample cells, detectors, instrumental wavelength and absorption calibration.</p> <p>e. Proton and Carbon NMR Spectroscopy: Theory of NMR, Instrumentation, Chemical shift, factors influencing chemical shift, solvents used in NMR, spin-spin splitting, coupling constant calculation, factors influencing coupling constant.</p> <p>f. Mass Spectrometry: Principle, Instrumentation and various</p>	20

	<p>fragmentation patterns.</p> <p>g. Conjoint spectrometry problems: Structural elucidation of organic molecules using IR, UV, NMR and MS.</p> <p>h. Raman Spectroscopy: Theory, Basic instrumentation and Structural analysis using Raman Spectra.</p> <p>(Note: Assignment based on all above spectrometric methods should be given to student. More weightage of lectures shall be given for solving IR and NMR data problems for structure elucidation)</p>	
<b>Pedagogy:</b>	<p>Mainly lectures and tutorials. Seminars / term papers / assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.</p>	
<b>References / Readings:</b>	<ol style="list-style-type: none"> <li>1. G. D. Christian, Analytical Chemistry, 6<sup>th</sup> Ed.; Wiley, 2004.</li> <li>2. J. H. Kennedy, Analytical Chemistry: Principles, 2<sup>nd</sup> Ed.; Saunders College Publishing, 1990.</li> <li>3. G. W. Ewing, Instrumental Methods of Chemical Analysis, 5<sup>th</sup> Ed.; McGraw- Hill Int., 1985.</li> <li>4. W. Kemp, Organic Spectroscopy, 3<sup>rd</sup> Ed.; Palgrave, 1991.</li> <li>5. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamentals of Analytical Chemistry, 9<sup>th</sup> Ed.; Cengage learning, 2014.</li> <li>6. F. J. Holler, D. A. Skoog, S. R. Crouch, Principles of Instrumental Analysis, 6<sup>th</sup> Ed.; Thomson Books, 2007.</li> <li>7. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental methods of Analysis, 7<sup>th</sup> Ed.; HCBS Publishing, 2004.</li> <li>8. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> Ed.; Tata McGraw- Hill, 2006.</li> <li>9. R. M. Silverstein, F. X. Webster, Spectrometric identification of Organic Compounds, 6<sup>th</sup> Ed.; Wiley, 1998.</li> <li>10. H. Gunzler, A. Williams, Handbook of Analytical Techniques, 1<sup>st</sup> Ed.; Wiley, 2001.</li> <li>11. P. S. Kalsi, Spectroscopy of Organic Compounds, 2<sup>nd</sup> Ed.; New Age International, 2000.</li> <li>12. E. Pretsch, P. Buhlmann, C. Affolter, Structural Determination of Organic Compounds, 2<sup>nd</sup> Ed.; Springer, 2005.</li> <li>13. L. D. Field, S. Sternhell, J. R. Kalman; Organic Structures from Spectra, 4<sup>th</sup> Ed.; Wiley, 2007.</li> <li>14. R. A. Day, A. L. Underwood, Quantitative Analysis, 6<sup>th</sup> Ed.; Prentice Hall, 2001.</li> <li>15. B. K Sharma, Instrumental methods of chemical analysis, Goel Publishing House, Meerut, 2004.</li> <li>16. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, 6<sup>th</sup> Ed.; Wiley, 2009.</li> <li>17. P. J. Larkin, Infrared and Raman Spectroscopy: principles and</li> </ol>	

	<p>spectral interpretation, 2<sup>th</sup> Ed.; Elsevier, 2018.</p> <p>18. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel's Text Book of Quantitative Chemical Analysis, 6<sup>th</sup> Ed.; Pearson, 2009.</p>
<b>Course outcomes:</b>	<ol style="list-style-type: none"><li>1. Students will be able to analyse the role of statistical tools for determination of error and organised data management for systematic interpretation.</li><li>2. Student will be able to apply the sampling and calibration methods for obtaining reliable results.</li><li>3. Students will be able to understand basic principles and scope of different methods of Analysis</li><li>4. Students will be able to solve problems based on IR, NMR, MS combined spectral data.</li></ol>

Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHA-521      Title of the course: Practical Course in Analytical Chemistry - I

Number of Credits: 02

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied chemistry practical courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
<b>Course Objectives:</b>	1. Introduction of various experimental techniques for analysis. 2. Learning data analysis, handling and interpretation of spectra.	
<b>Content:</b>	<i>This course consists of 7 units of experiments in various areas of Analytical chemistry. Minimum 13 experiments which include at least 02 experiments from unit 1-6 and 01 experiment from unit 7 shall be conducted.</i>	No of hours
	<b>Unit 1: Statistics</b> i. Calibration of selected Volumetric apparatus ii. Calibration of selected Laboratory instruments Preparation of standard solutions and standardisation.	9
	<b>Unit 2: Colorimetry/ UV-Visible Spectrophotometry</b> i. Estimation of Iron from Pharmaceutical sample (capsule) by thiocyanate method ii. Estimation of phosphoric acid in cola drinks by molybdenum blue method. iii. Estimation of $\text{KNO}_3$ by UV spectroscopy and $\text{K}_2\text{Cr}_2\text{O}_7$ by Visible spectroscopy iv. Simultaneous determination and Verification of law of additivity of absorbances ( $\text{K}_2\text{Cr}_2\text{O}_7$ and $\text{KMnO}_4$ ).	8
	<b>Unit 3: Flame Spectrophotometry and AES/AAS/ICP Spectroscopy</b> i. Estimation of Na and K in food supplements or cosmetic products. ii. Estimation of Pb in water sample by AES/AAS/ICP. iii. Estimation of Fe and Al in Iron ore sample by AES/AAS/ICP.	9
	<b>Unit 4: Ion Exchange Chromatography and High Pressure Liquid Chromatography</b> i. Separation and Estimation of chloride and bromide. ii. Separation of Anthracene and Naphthalene using reverse phase chromatography iii. Separation of Benzaldehyde and Benzyl alcohol using normal phase chromatography	10



	<p><b>Unit 5: Volumetric Titrations</b></p> <ul style="list-style-type: none"> <li>i. Estimation of Ca in pharmaceutical tablet.</li> <li>ii. Estimation of Al and Mg in antacid tablet.</li> <li>iii. Estimation of CaO in cement.</li> </ul>	10
	<p><b>Unit 6: Solvent Extraction and spectrophotometry</b></p> <ul style="list-style-type: none"> <li>i. Extraction of Cu as copper dithiocarbamate (DTC) using solvent extraction and estimation by spectrophotometry.</li> <li>ii. Determination of Ni as Dimethylglyoxime complex by spectrophotometry.</li> <li>iii. Determination of Silver as ion association complex with 1,10-Phenanthroline and Bromopyrogallol red.</li> </ul>	10
	<p><b>Unit 7: Interpretation Exercises</b></p> <ul style="list-style-type: none"> <li>i. Thermal studies: TG/DTA and Isothermal weight loss studies of various hydrated solids like <math>\text{CuSO}_4 \cdot 5\text{H}_2\text{O}</math>, <math>\text{Ca}_2\text{C}_2\text{O}_4 \cdot \text{H}_2\text{O}</math>, <math>\text{Fe}_2\text{C}_2\text{O}_4 \cdot 2\text{H}_2\text{O}</math>.</li> <li>ii. X-ray powder diffractometry: Calculation of lattice parameters from X-ray powder pattern of cubic system such as <math>\text{NiMn}_2\text{O}_4</math>, <math>\text{CoFe}_2\text{O}_4</math> etc.</li> <li>iii. IR spectra of Urea, benzoic acid, Copper sulphate pentahydrate etc.</li> </ul>	4
<b>Pedagogy:</b>	Prelab exercises / assignments / presentations / lab hand-out or a combination of some of these. Sessions shall be interactive in nature to enable peer group learning.	
<b>References / Readings:</b>	<ol style="list-style-type: none"> <li>1. J. H. Kennedy, Analytical Chemistry Principles, Saunders College Publishing, 2<sup>nd</sup> Ed., 1990.</li> <li>2. G. D. Christian, Analytical chemistry, 5<sup>th</sup>Ed., John Willey and Sons, 1994</li> <li>3. J. Mendham, R.C. Denney, J.D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis, 6<sup>th</sup>Ed., Pearson Education Asia 2009.</li> <li>4. A. J. Elias, Collection of interesting chemistry experiments, University press, 2002.</li> <li>5. R.A. Day &amp; A.L. Underwood, Quantitative Analysis, 6<sup>th</sup>Ed., Prentice Hall, 2001.</li> <li>6. J. Kenkel, Analytical Chemistry for Technicians, 3<sup>rd</sup>Ed., Lewis publishers, 2002.</li> </ol>	
<b>Course outcomes:</b>	<ol style="list-style-type: none"> <li>1. Students will be able to explain how to determine an unknown concentration of solution.</li> <li>2. Students will use statistical methods to analyse data in laboratory.</li> <li>3. Students will be able to use different techniques for qualitative and quantitative estimation.</li> <li>4. Students will be able to interpret TG/X-Ray/IR spectra.</li> </ol>	

Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHA-522 Title of the course: Practical Course in Analytical Chemistry - II

Number of Credits: 02

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied chemistry practical courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
<b>Course Objectives:</b>	1. Introduction of various experimental techniques for analysis. 2. Learning data analysis, handling and interpretation of spectra.	
<b>Content:</b>	<i>This course consists of 7 units of experiments in various areas of Analytical chemistry. Minimum 13 experiments which include at least 02 experiments from unit 1-6 and 01 experiment from unit 7 shall be conducted.</i>	No of hours
	<b>Unit 1: Statistics</b> i. Calibration of selected Volumetric apparatus ii. Calibration of selected Laboratory instruments iii. Preparation of standard solutions and standardisation.	9
	<b>Unit 2: Titrimetric Analysis</b> i. Standardisation and estimation of Chloride using precipitation titration (Mohr's method) ii. Analysis of commercial caustic soda by neutralisation titrimetric method iii. Determination of sulphates by complexometric titrations using EDTA.	8
	<b>Unit 3: Flame Spectrophotometry and AES/AAS/ICP Spectroscopy</b> i. Estimation of Na and K in food supplements or cosmetic products using flame photometer. ii. Estimation of chromium in water sample by AES/AAS/ICP. iii. Estimation of nickel, molybdenum in Hastelloy C-22 using AES/AAS/ICP.	10
	<b>Unit 4: Natural product isolation and Ion Exchange Chromatography</b> i. Isolation of cinnamaldehyde from cinnamon ii. Isolation of Caffeine from tea powder iii. Separation and estimation of Cadmium and Zinc	9
	<b>Unit 5: UV-Visible Spectrophotometry and High-Pressure Liquid Chromatography</b> i. Estimation of $\text{KNO}_3$ and $\text{K}_2\text{Cr}_2\text{O}_7$ using UV- Visible	10

	<p>spectroscopy</p> <p>ii. Separation of Benzaldehyde and benzoic acid using reverse phase HPLC.</p> <p>iii. Quantification of naphthalene in a sample using reverse phase HPLC.</p>	
	<p><b>Unit 6: Solvent Extraction and spectrophotometry</b></p> <p>i. Spectrophotometric determination of aspirin/phenacetin/caffeine in APC tablet using solvent extraction</p> <p>ii. Colorimetric determination of iron with salicylic acid.</p> <p>iii. Determination of copper in brass sample by colorimetry.</p>	10
	<p><b>Unit 7: Data Interpretation Exercises</b></p> <p>i. NMR/Mass spectra</p> <p>ii. HPLC and GC chromatograph</p> <p>iii. XRD powder pattern of cubic systems</p> <p>iv. Thermogram of coordination compounds</p>	4
<b>Pedagogy:</b>	<p>Pre-lab exercises / assignments / presentations / lab hand-out or a combination of some of these. Sessions shall be interactive in nature to enable peer group learning.</p>	
<b>References / Readings:</b>	<ol style="list-style-type: none"> <li>1. J. H. Kennedy, Analytical Chemistry Principles, Saunders College Publishing, 2<sup>nd</sup> Ed., 1990.</li> <li>2. G. D. Christian, Analytical chemistry, 5<sup>th</sup> Ed., John Wiley and Sons, 1994</li> <li>3. J. Mendham, R.C. Denney, J.D. Barnes, M. Thomas, B. Sivasankar, Vogel's Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> Ed., Pearson Education Asia 2009.</li> <li>4. J. Elias, Collection of interesting chemistry experiments, University press, 2002.</li> <li>5. R.A. Day &amp; A.L. Underwood, Quantitative Analysis, 6<sup>th</sup> Ed., Prentice Hall, 2001.</li> <li>6. J. Kenkel, Analytical Chemistry for Technicians, 3<sup>rd</sup> Ed., Lewis publishers, 2002.</li> </ol>	
<b>Course outcomes:</b>	<ol style="list-style-type: none"> <li>1. Students will be able to standardize a material to determine an unknown concentration.</li> <li>2. Students will use statistical methods to analyse data in laboratory.</li> <li>3. Students will be able to use different techniques for qualitative and quantitative estimation.</li> <li>4. Students will be able to interpret TG/X-Ray/IR spectra.</li> </ol>	

Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHI-500 Title of the course: Fundamentals of Inorganic Chemistry

Number of Credits: 04

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied chemistry courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University	
<b>Course Objective:</b>	1.To introduce atomic structure, molecular structure, bonding, and symmetry. 2.To provide fundamental knowledge of solid state chemistry, coordination chemistry, organometallic chemistry, and bioinorganic chemistry. 3.To provide fundamental aspects of transition & inner transition elements & their compounds. 4.To introduce air and water pollution, and its treatments, to follow directive of the Supreme Court in 1993 to introduce environmental education at all levels.	
<i>Content</i>	<b>1. Atomic structure, molecular structure and bonding</b> a. Atomic Structure: Structures of hydrogenic atoms: some principles of quantum mechanics, atomic orbitals. Many electron atoms: penetration & shielding, building up principle, classification of elements. Spectroscopic terms. Atomic properties: atomic radii, ionic radii, ionization energy, electron affinity, electronegativity, polarizability. b. Molecular Structure & bonding: Lewis structures: octet rule, resonance. VSEPR model: basic shapes, modification of the basic shapes. Valence bond theory: hydrogen molecule, homonuclear diatomic molecules, polyatomic molecules, promotion, hypervalence, hybridization. Molecular orbital theory: approximation, bonding & antibonding orbitals. Homonuclear diatomic molecules & Heteronuclear diatomic molecules	No of hours  10
	<b>2. Molecular Symmetry</b> a. Symmetry elements and symmetry operations. b. Equivalent symmetry elements and equivalent atoms, symmetry point groups with examples, point groups of higher symmetry. c. Systematic procedure for symmetry classification of molecules and illustrative examples, dipole moment, optical activity and point groups	4
	<b>3. Solid state chemistry</b> a. Structures of solids: crystal structures, lattices and unit cells,	10

	<p>fractional atomic coordinates and projections, close packing of spheres, holes in closed-packed structures.</p> <p>b. Structures of metals &amp; alloys: polytypism, nonclosed-packed structures, polymorphism of metals, atomic radii of metals, alloys, substitutional and interstitial solid solutions, intermetallic compounds.</p> <p>c. Ionic solids: characteristic structures of ionic solids, binary phases, ternary phases, rationalization of structures, ionic radii, radius ratio, structure maps, energetics of ionic bonding, lattice energy and the Born–Haber cycle, The calculation of lattice enthalpies. (numerical expected)</p>	
	<p><b>4. Chemistry of transition &amp; inner transition elements</b></p> <p>a. Transition elements: IUPAC definition of transition elements, occurrence, physical and chemical properties, noble character, metal halides, oxides &amp; oxido complexes, examples of metal-metal bonded clusters, difference between 1<sup>st</sup> row and other two rows.</p> <p>b. Inner transition elements: Lanthanides, occurrence, properties, oxidation states, electronic structure, colour and spectra, magnetic properties, lanthanide contraction, compounds of lanthanides. Actinoid chemistry: general trends and properties, electronic spectra, thorium and uranium.</p>	10
	<p><b>5. Coordination and Organometallic Chemistry</b></p> <p>a. Coordination chemistry: Introduction, representative ligands, nomenclature. Constitution and geometry: low coordination numbers, intermediate coordination numbers, higher coordination numbers, polymetallic compounds. Isomerism &amp; chirality in square planar and octahedral complexes, ligand chirality. Thermodynamics of complex formation: formation constants, chelate and macrocyclic effects, steric effects and electron delocalization. Electronic properties of metal complexes: CFT applied to octahedral and tetrahedral complexes, magnetic moments, CFSE. Electronic spectroscopy: basic concepts, interpretation of spectra of d<sup>1</sup> &amp; d<sup>9</sup> ions (Orgel diagram for octahedral and tetrahedral complexes).</p> <p>b. Organometallic Chemistry: Introduction to organometallic chemistry, nomenclature, stability and inert gas rules (neutral atom and donor pair electron count methods). Ligands: CO &amp; phosphines, homoleptic carbonyls its synthesis and properties, oxidation-reduction of carbonyls, metal carbonyl basicity, reactions of CO ligand, spectroscopic properties of metal carbonyls. Oxidative addition and reductive elimination.</p>	12
	<p><b>6. Basic Bioinorganic Chemistry</b></p> <p>a. Macronutrients/micronutrients. Role of elements in biology.</p>	4

	<p>Metal ion transport role.</p> <p>b. Definition of metallobiomolecules, metalloporphyrins, structure of porphine and heme group, examples of metalloenzymes of Cu and Zn.</p>	
	<p><b>7. Environmental Chemistry</b></p> <p>a. Air Pollution: Classification of air pollutants and photochemical reactions in the atmosphere. Common air pollutants (e.g. CO, NO<sub>x</sub>, SO<sub>2</sub>, hydrocarbons and particulates) (a) sources (b) physiological and environmental effect (c) monitoring, (d) various remedial &amp; technological measures to curb pollution. Air quality standards.</p> <p>b. Water pollution: Importance of buffer &amp; buffer index in waste water treatments. Chemical, physical &amp; biological characteristics of water pollution, specific &amp; non-specific characterization of water. DO, BOD, COD, and chlorine demand, typical water treatment &amp; waste water treatment (Municipal). Impact of plastic pollution and its effect.</p>	10
<b>Pedagogy</b>	<p>Mainly lectures and tutorials. Seminars / term papers / assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.</p>	
<b>References / Readings:</b>	<ol style="list-style-type: none"> <li>1. P. W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Shriver &amp; Atkins Inorganic Chemistry, 5<sup>th</sup> Ed.; Oxford Publications, 2009.</li> <li>2. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure &amp; Reactivity, 4<sup>th</sup> Ed.; Pearson, 2011.</li> <li>3. F. A. Cotton, G. Wilkinson, P. L. Gaus, Basic Inorganic Chemistry, 3<sup>rd</sup> Ed.; Wiley, 2008 (reprint).</li> <li>4. J. D. Lee, Concise Inorganic Chemistry, 5<sup>th</sup> Ed.; Wiley, 2008.</li> <li>5. F. A. Cotton, Chemical applications of group theory, 3<sup>rd</sup> Ed.; Wiley Eastern, 2012 (reprint).</li> <li>6. L. Pauling, The Nature of The Chemical Bond, 3<sup>rd</sup> Ed.; Cornell University Press, 1960.</li> <li>7. M. C. Day, J. Selbin, Theoretical Inorganic Chemistry, 2<sup>ed</sup> Ed.; Van Nostrand-Reinhold, 1969.</li> <li>8. H. V. Keer, Principles of Solid state Chemistry, 1<sup>st</sup> Ed.; New Age Intl. Ltd, 1993, (reprint 2008).</li> <li>9. A. R. West, Solid State Chemistry and Its Applications, 1<sup>st</sup> Ed.; John Wiley &amp; Sons, Singapore, 1984 (reprint 2007).</li> <li>10. D. K. Chakrabarty, Solid State Chemistry, 2<sup>ed</sup> Ed.; New Age Intl. Publishers, 2010.</li> <li>11. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 3<sup>rd</sup> Ed.; Wiley Eastern, 2001.</li> <li>12. A. V. Salker, Environmental Chemistry: Pollution and Remedial Perspective, 1<sup>st</sup> Ed.; Narosa Publication, 2017.</li> </ol>	

	<p>13. A.K. De, Environmental Chemistry, 3<sup>rd</sup> Ed.; New Age Intl. Publishers, 2005.</p> <p>14. A. C. Stern, R. W. Boubel, D. Bruce turner, D. L. Fox, Fundamentals of Air Pollution, 1<sup>st</sup> Ed.; Academic Press, 1984.</p> <p>15. R. A. Horne, Chemistry of Our Environment, 1<sup>st</sup> Ed.; John Wiley, 1978.</p> <p>16. R. S. Drago, Physical Methods in Inorganic Chemistry, Affiliated East West Press Pvt. Ltd., 2017</p> <p>17. G. C. Miessler, D. A. Tarr, Inorganic Chemistry, 3<sup>rd</sup> Ed.; Pearson, 2004</p>
<p><b>Course outcomes:</b></p>	<ol style="list-style-type: none"> <li>1. Students will be able to predict geometry and shape of different molecules, and the point group symbols.</li> <li>2. Students will be able to explain the fundamentals of atomic and molecular structure, solid state chemistry, coordination chemistry, organometallic chemistry, and bioinorganic chemistry.</li> <li>3. Students should be able to describe and explain the properties and usefulness of transition &amp; inner transition metals.</li> <li>4. Students will able to explain different air and water pollutants and will be in a position to apply knowledge to treat these pollutants.</li> </ol>

Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHI-521 Title of the course: Practical course in Inorganic Chemistry-I

Number of Credits: 02

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied chemistry practical courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
<b>Course Objective:</b>	1. Students shall acquire skills in synthetic inorganic chemistry. 2. Students will learn to prepare coordination compounds. 3. Students will learn to prepare useful potash alum from scrap aluminum. 4. Students will learn how to grow single crystals. 5. Students will acquire skills in determination of chromium, oxalate, and aluminum by redox titrations. 6. Students will be trained to fix the formula of compounds and find lattice water molecules by complexometric, redox & iodometric titrations. 7. Students shall acquire skills in determination of metal content at very low concentrations (ppm) using colorimetry / spectrophotometry.	
<b>Content</b>	<i>Minimum 13 experiments from the list shall be conducted.</i> <b>1. Preparations / Synthesis of Inorganic Compounds: (Any Five)</b> i. Preparation of hexaamminenickel(II) chloride. ii. Preparation of Trisethylenediaminecobalt(III) chloride. iii. Preparation of potassium trioxalatoaluminate trihydrate. iv. Preparation of potassium hexathiocyanato- $\kappa N$ -chromate tetrahydrate. v. Preparation of potassium trioxalatochromate trihydrate. vi. Preparation of potash alum from scrap aluminum.	No of hours  25
	<b>2. Estimations / Determinations: (Any Eight)</b> i. Estimation of nickel in $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$ by complexometry or Gravimetry. ii. Estimation of cobalt in $[\text{Co}(\text{en})_3]\text{Cl}_3$ by complexometry. iii. Estimation of oxalate in $\text{K}_3[\text{Al}(\text{C}_2\text{O}_4)_3]\cdot x\text{H}_2\text{O}$ or $\text{K}_3[\text{Cr}(\text{C}_2\text{O}_4)_3]\cdot x\text{H}_2\text{O}$ iv. Estimation of nitrite by redox titration. v. Estimation of calcium from calcite ore. vi. Iodometric determination of Copper in gun metal alloy/Devarda's alloy. vii. Determination of chromium in chrome alum and $\text{K}_3[\text{Cr}(\text{C}_2\text{O}_4)_3]\cdot x\text{H}_2\text{O}$ and to determine degree of hydration. viii. Colorimetric/Spectrophotometric determination of nickel or	35



	chromium. ix. Estimation of manganese by colorimetric / spectrophotometry method.	
<b>Pedagogy</b>	Students will be given pre-lab and post-lab assignments on theoretical aspects of laboratory experiments prior to the conduct of each experiment. Exams will be in the form of ISA, SEA which will involve performing given experiments and conduct of viva, systematic reporting of experiments, results and observations in laboratory report. Sessions should be interactive in nature to enable peer group learning.	
<b>References / Readings</b>	<ol style="list-style-type: none"> <li>1. G. Brauer, Handbook of Preparative Inorganic Chemistry, Vol. 1 &amp; 2, 1963.</li> <li>2. G. Pass &amp; H. Sutcliffe, Practical Inorganic Chemistry, Preparations, Reactions and Instrumental Methods, 2<sup>nd</sup> Ed.; Chapman &amp; Hall, 1974.</li> <li>3. S. De Meo, J. Chem. Ed., Vol 80, Pg.No.796-798, 2003.</li> <li>4. W. L. Jolly, The Synthesis &amp; Characterization of Inorganic Compounds, Prentice-Hall, INC, 1970.</li> <li>5. A. J. Elias, General Chemistry Experiments, Revised Ed.; University Press, 2008.</li> <li>6. J. Mendham, R.C. Denney, J.D. Barnes, M.J. K. Thomas, Vogel's Text Book of Quantitative Chemical Analysis, 6<sup>th</sup> Ed.; Pearson, 2002.</li> <li>7. G. Svehla, Vogel's Text Book of Qualitative Inorganic Analysis, 7<sup>th</sup> Ed, Pearson, 2011.</li> <li>8. G. Marr, B. W. Rockett, Practical Inorganic Chemistry, Van Nostrnad Reinhold London, 1972.</li> </ol>	
<b>Course outcomes:</b>	<ol style="list-style-type: none"> <li>1. Students will be in a position to synthesis coordination compounds with different metals and ligands.</li> <li>2. Students will be able to grow single crystal.</li> <li>3. Students will be able to prepare potash alum compound from waste scrap Al source.</li> <li>4. Students will be able to determine metal content in the synthesised inorganic compounds.</li> <li>5. Students will be able to fix the formula of compounds.</li> <li>6. Students will be able to use and explain the diverse methods available for estimation of the metals including colorimeters and spectrometers.</li> </ol>	

Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHI-522 Title of the course: Practical course in Inorganic Chemistry-II

Number of Credits: 02

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied chemistry practical courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
<b>Course Objective:</b>	<ol style="list-style-type: none"><li>1. Students shall acquire skills in synthetic inorganic chemistry.</li><li>2. Students will learn to prepare coordination compounds.</li><li>3. Students will learn how to grow single crystals.</li><li>4. Students will acquire skills in determination of metal present by gravimetric and titrimetric method.</li><li>5. Students shall acquire skills in determining the metal content at very low concentrations (ppm) using colorimetry / spectrophotometry.</li></ol>	
<b>Content</b>	<p><i>Minimum 13 experiments from the list shall be conducted.</i></p> <p><b>1. Preparations / Estimation of Inorganic Compounds: (Any Nine)</b></p> <ol style="list-style-type: none"><li>i. Preparation of hexaamminecobalt(III) nitrate.</li><li>ii. Estimation of cobalt in hexaamminecobalt(III) nitrate by volumetric titration.</li><li>iii. Preparation of Potassium Trioxalatoferate(III) Trihydrate</li><li>iv. Estimation of iron and oxalate by redox titration</li><li>v. Synthesis of metal nanoparticles (Cu, Ag, Au, Ni) and determining the absorption maxima by UV-visible spectrophotometer.</li><li>vi. Estimation of amount of calcium in given sample by gravimetric method.</li><li>vii. Estimation of amount of nickel in given sample by gravimetric method.</li><li>viii. Estimation amount of zinc present in given sample by gravimetric method.</li><li>ix. Estimation of iron by colorimetric / spectrophotometry method.</li><li>x. Estimation of barium by complexometric titration method.</li><li>xi. Estimation of manganese in presence of iron by complexometric titration method.</li></ol>	No of hours  40
	<p><b>2. Semi-micro qualitative analysis of cation and anion in a given inorganic mixture: (Any four mixture)</b></p> <p>Mixture containing total six cations and/or anions. <b>Cations :</b> <math>\text{Pb}^{2+}</math>, <math>\text{Cu}^{2+}</math>, <math>\text{Cd}^{2+}</math>, <math>\text{Sn}^{2+}</math>, <math>\text{Fe}^{2+}</math>, <math>\text{Fe}^{3+}</math>, <math>\text{Al}^{3+}</math>, <math>\text{Cr}^{3+}</math>, <math>\text{Zn}^{2+}</math>,</p>	20

	$Mn^{2+}, Ni^{2+}, Co^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}, (NH_4)^+, K^+$ <b>Anions:</b> $Cl^-, Br^-, I^-, NO_2^-, NO_3^-, SO_3^{2-}, CO_3^{2-}, SO_4^{2-}, PO_4^{3-}, S^{2-}$
<b>Pedagogy</b>	Students will be given pre-lab and post-lab assignments on theoretical aspects of laboratory experiments prior to the conduct of each experiment. Exams will be in the form of ISA, SEA which will involve performing given experiments and conduct of viva, systematic reporting of experiments, results and observations in laboratory report. Sessions should be interactive in nature to enable peer group learning.
<b>References / Readings</b>	<ol style="list-style-type: none"> <li>1. G. Brauer, Handbook of Preparative Inorganic Chemistry, Vol. 1 &amp; 2, 1963.</li> <li>2. G. Pass &amp; H. Sutcliffe, Practical Inorganic Chemistry, Preparations, Reactions and Instrumental Methods, 2<sup>nd</sup> Ed.; Chapman &amp; Hall, 1974.</li> <li>3. S. De Meo, J. Chem. Ed., Vol 80, Pg.No.796-798, 2003.</li> <li>4. W. L. Jolly, The Synthesis &amp; Characterization of Inorganic Compounds, Prentice-Hall, INC, 1970.</li> <li>5. A. J. Elias, General Chemistry Experiments, Revised Ed.; University Press, 2008.</li> <li>6. J. Mendham, R.C. Denney, J.D. Barnes, M.J. K. Thomas, Vogel's Text Book of Quantitative Chemical Analysis, 6<sup>th</sup> Ed.; Pearson, 2002.</li> <li>7. G. Svehla, Vogel's Text Book of Qualitative Inorganic Analysis, 7<sup>th</sup> Ed, Pearson, 2011.</li> <li>8. G. Marr &amp; B. W. Rockett, Practical Inorganic Chemistry, Van Nostrand Reinhold Company, London, 1972.</li> </ol>
<b>Course outcomes:</b>	<ol style="list-style-type: none"> <li>1. Students will be in a position to synthesize coordination compounds with different metals and ligands.</li> <li>2. Students will be able to grow single crystal.</li> <li>3. Students will be able to determine metal content in the given sample.</li> <li>4. Students will be in position to apply diverse methods available for estimation of the metals and can use colorimeters and spectrometers.</li> <li>5. Students will be able to detect cations and anions in the given salt.</li> </ol>

Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHO-500 Title of the course: Fundamentals of Organic Chemistry

Number of Credits: 04

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied chemistry courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
<b>Course Objective:</b>	1. To study the various concepts based on molecular orbital theory. 2. To understand the concepts of topicity, prostereoisomerism and chemo-, regio- and stereoselectivity in organic reactions. 3. To understand the mechanistic aspects of various type of reactions in organic synthesis.	
<b>Content</b>	<b>1.Molecular orbitals and delocalized chemical bonding</b> a. Qualitative description of molecular orbitals of simple acyclic and monocyclic systems, frontier molecular orbitals. b. Conjugation, cross conjugation, resonance, hyperconjugation and tautomerism (types and examples). c. Aromaticity: Origin of Huckel's rule, examples of aromatic, non-aromatic and antiaromatic compounds; concept of Mobius aromaticity.	No of hours  08
	<b>2. Structure &amp; Reactivity</b> a. Acidity, basicity and pKa of organic compounds; Acid and base strengths; HSAB concept & Factors affecting it, effect of structure & medium on acid and base strength. b. Concept of superacids and superbases. c. Electrophilicity & nucleophilicity, examples of ambident nucleophiles & electrophiles. (Including revision of aromatic electrophilic and nucleophilic substitution)	08
	<b>3. Stereochemistry</b> a. Brief revision of configurational nomenclature: R & S; D & L; E & Z; cis & trans and <i>syn</i> & <i>anti</i> nomenclature. Chirality in molecules with two and more chiral centres. b. Conformational analysis of open chain compounds (Butane, 2, 3-butane diol, 2,3-dibromobutane etc.). <i>Erythro</i> and <i>threo</i> nomenclature. c. Topicity and Prostereoisomerism: Topicity of ligands and faces-homotopic, enantiotopic and Cram's rule /diastereotopic ligands and faces. d. Introduction to chemoselective, regioselective and	14

	<p>stereoselective reactions.</p> <p>e. Stereochemistry of <i>cis</i>- and <i>trans</i>-decalins, conformation and reactivity of cyclohexane and substituted cyclohexanes, cyclohexene / cyclohexanone. conformational isomerism and analysis in acyclic and simple cyclic systems –substituted ethanes, cyclopentane, cyclohexane cycloheptane, cyclooctane and decalins,</p> <p>f. optical isomerism - optical activity - molecular dissymmetry and chirality - elements of symmetry. optical isomerism in biphenyls, allenes and spirans - optical isomerism of nitrogenous compounds racemisation and resolution.</p>	
	<p><b>4.Reaction Mechanism</b></p> <p>a. Brief revision of carbocations, carbanions, free radicals, carbenes, Arynes and nitrenes with reference to generation, structure, stability and reactivity;</p> <p>b. Types of mechanisms, types of reactions, thermodynamic and kinetic control.</p> <p>c. The Hammond postulate and principle of microscopic reversibility,</p> <p>d. Methods of determining reaction mechanisms like-</p> <p>i. Identification of products,</p> <p>ii. Determination of the presence of intermediates (isolation, detection, trapping and addition of suspected intermediate,</p> <p>iii. Isotopic labelling,</p> <p>iv. Stereochemical evidence,</p> <p>v. Kinetic evidence and</p> <p>vi. Isotope effect (at least two reactions to exemplify each method be studied)</p>	08
	<p><b>5.Aliphatic Nucleophilic substitution</b></p> <p>a. Brief revision of nucleophilic substitutions with respect to Mechanism, various factors affecting such reactions;</p> <p>b. The Neighbouring Group Participation (NGP)/ Anchimeric assistance: General approach to various NGP processes; NGP by unshared/lone pair of electrons; NGP by <math>\pi</math>-electrons; NGP by aromatic rings (formation of phenonium ion intermediate); NGP by sigma bonds with special reference to bornyl and nor-bornyl system (formation of nonclassical carbocation)</p>	08
	<p><b>6.Elimination reactions</b></p> <p>a. The E2, E1 and E1cB mechanisms. Orientation of the double bond, Saytzeff and Hofmann rule.</p> <p>b. Effects of changes in the substrate, base, leaving group and medium on</p>	08

	<p>i. Overall reactivity,  ii. E1 vs. E2 vs. E1cB  iii. Elimination vs substitution, Mechanism and orientation in pyrolytic <i>syn</i> elimination (various examples involving cyclic and acyclic substrates to be studied).</p>	
	<p><b>7. Selective reagents for Organic transformation</b>  a. Oxidation of organic compounds, PCC, PDC and MnO<sub>2</sub>, ozonolysis, peracids.  b. Reduction of organic compounds: NaBH<sub>4</sub>, LAH, DIBAL reduction and reduction with borane and dialkylboranes. Clemmensen reduction, Birch reduction and Wolff-Kishner reduction</p>	06
<b>Pedagogy</b>	Mainly lectures and tutorials. Seminars/term papers/assignments/presentations/ self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
<b>References / Readings</b>	<ol style="list-style-type: none"> <li>1. W. Caruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 4<sup>th</sup> Ed., 2016.</li> <li>2. M. B. Smith, Organic Synthesis, McGraw-HILL, New York, International Edition, 1994.</li> <li>3. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2<sup>nd</sup> Ed., 2012.</li> <li>4. R. Bruckner, Advanced Organic Chemistry – Reaction Mechanisms, San Diego, CA: Harcourt /Academic Press, San Diego, 2002.</li> <li>5. J. Fuhrhop, G. Penxlin, Organic Synthesis – Concepts, Methods, Starting Materials, VCH Publishers Inc., New York, 1994.</li> <li>6. H. O. House, Modern Synthetic Reactions, W. A. Benjamin, 2<sup>nd</sup>Ed.,1965</li> <li>7. M. Nogradi, Stereoselective Synthesis, VCH Publishers, Inc., Revised and Enlarged Edition, 1994.</li> <li>8. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Springer India Private Limited, 5<sup>th</sup>Ed, 2007.</li> <li>9. T. Laue, A. Plagens, Named Organic Reactions, John Wiley and Sons, Inc., 2005.</li> </ol>	
<b>Course outcomes:</b>	<ol style="list-style-type: none"> <li>1. Students will be in a position to evaluate the effect of delocalization of electrons &amp; presence or absence of aromaticity in organic compounds.</li> <li>2. Students will be able to apply various concepts in stereochemistry to understand stereochemical outcome in a reaction.</li> <li>3. Students shall be in a position to understand/propose plausible mechanism of organic reactions.</li> <li>4. Students will understand and apply various reagents for desired organic transformations.</li> </ol>	

Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHO-521      Title of the course: Practical Course in Organic Chemistry-I

Number of Credits: 02

Effective from AY: 2022-23

<b>Prerequisites for the course</b>	Students should have studied chemistry practical courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
<b>Course Objective:</b>	To translate certain theoretical concepts learnt earlier into experimental knowledge by providing hands on experience of basic laboratory techniques required for organic syntheses.	
<b>Content</b>	<i>Minimum 13 experiments from the list shall be conducted.</i> <b>1. Introduction to laboratory equipments, apparatus and safety</b> a. Use of common laboratory equipments like fume hoods, vacuum pumps, weighing balance etc. to be explained to the students. b. Introduction to various types of quick fit joints and apparatus to the students. c. Discussion of Safety Techniques: i Disposal of chemicals ii Usage of protective equipment's iii First aid iv Fire extinguishers, types of fire v Hazards of chemicals and risk assessment	No of hours 04
	<b>2. Laboratory Techniques</b> a. Simple distillation (any one): i. Toluene-dichloromethane mixture using water condenser. ii. Nitrobenzene and aniline using air condenser. b. Steam distillation (anyone): i. Separation of <i>o</i> - and <i>p</i> - nitrophenols. ii. Naphthalene from its suspension in water, iii. Clove oil from cloves. c. Crystallisation: Concept of induction of crystallization (any one) i. Crystallisation of phthalic acid from hot water using fluted filter paper and stemless funnel. ii. Acetanilide from boiling water iii. Naphthalene from ethanol. iv. Decolorisation and crystallization of brown sugar (sucrose) with animal charcoal using gravity filtration. d. Sublimation: Simple or vacuum sublimation of camphor, naphthalene, anthracene or succinic acid (any one). e. Vacuum distillation (any one): <i>o</i> -dichlorobenzene, diphenyl	24

	<p>ether. Also use of nomograph should be explained.</p> <p>f. Thin layer Chromatography (any one):</p> <p>i. Separation of <i>o</i> and <i>p</i>-nitroanilines.</p> <p>ii. Separation of analgesic drugs</p> <p>iii. Separation of <i>o</i> and <i>p</i>-nitrophenols,</p>	
	<p><b>3. Organic synthesis (Any Seven experiments)</b></p> <p>a. Aliphatic electrophilic substitution: Preparation of iodoform from ethanol &amp; acetone.</p> <p>b. Aromatic electrophilic substitution (any one):</p> <p>i. Preparation of <i>p</i>-bromoacetanilide.</p> <p>ii. Bromination of acetophenone to phenacyl bromide</p> <p>iii. Nitration of naphthalene to 1-nitronaphthalene</p> <p>iv. Nitration of benzaldehyde to 3-nitrobenzaldehyde.</p> <p>c. Oxidation (any one)</p> <p>i. Benzoic acid from toluene.</p> <p>ii. Cyclohexanone from cyclohexanol.</p> <p>iii Isoborneol to camphor using Jones reagent.</p> <p>d. Reduction (any one)</p> <p>i. Reduction of <i>o</i>-nitroaniline to <i>o</i>-phenylenediamine using Sn/HCl</p> <p>ii. Reduction of <i>p</i>-nitro benzaldehyde to <i>p</i>-nitrobenzyl alcohol using NaBH<sub>4</sub>.</p> <p>e. Bromination of an alcohol using CBr<sub>4</sub>/ triphenylphosphine.</p> <p>f. Grignard reaction: Triphenylmethanol from benzoic acid ester or benzophenone.</p> <p>g. Aldol condensation: Dibenzal acetone from benzaldehyde</p> <p>h. Acetoacetic ester condensation: Preparation of ethyl <i>n</i>-butylacetoacetate or ethyl acetoacetate.</p> <p>i. Cannizzaro reaction using 4-chlorobenzaldehyde as substrate.</p> <p>j. Friedel Craft's reaction (any one):</p> <p>i. using toluene and succinic anhydride</p> <p>ii. Resorcinol to resacetophenone, benzene and maleic anhydride to <math>\beta</math>-benzoylacrylic acid</p> <p>k. Solvent free preparation of coumarin by the Knoevenagel condensation under MW irradiation.</p> <p>l. Preparation of oxidizing agent (any one): Pyridinium chlorochromate-silica, pyridinium chlorochromate-alumina, MnO<sub>2</sub>.</p> <p>m. Preparation of cuprous chloride.</p>	24
	<p><b>4. Isolation from natural sources (Any two)</b></p> <p>i. Caffeine from tea powder.</p> <p>ii. Piperine from pepper.</p> <p>iii. Cinnamaldehyde from cinnamon</p> <p>iv. Lemongrass oil from lemongrass</p>	8
<b>Pedagogy:</b>	Students should be given suitable pre- and post-lab assignments	



	and explanation revising the theoretical aspects of laboratory experiments prior to the conduct of each experiment. Each of the experiments should be done individually by the students.	
<b>References / Readings</b>	<ol style="list-style-type: none"> <li>1. A.I. Vogel, A., R. Tatchell, B. S. Furniss, A.J. Hannaford, Vogel's Textbook of Practical Organic Chemistry, 5<sup>th</sup>Ed., Prentice Hall; 2011.</li> <li>2. D. Pasto, C. Johnson and M. Miller, Experiments and Techniques in Organic Chemistry, 1<sup>st</sup>Ed., Prentice Hall, 1991.</li> <li>3. L.F. Fieser, K.L. Williamson, Organic Experiments, 7<sup>th</sup>edition D. C. Heath, 1992.</li> <li>4. K.L. Williamson, K.M. Masters, Macroscale and Microscale Organic Experiments, 6<sup>th</sup>Edition, Cengage Learning, 2010</li> <li>5. R.K. Bansal, Laboratory Manual in Organic Chemistry, New Age International, 5<sup>th</sup>Edition, 2016.</li> <li>6. S. Delvin, Green Chemistry, Sarup &amp; Sons, 2005.</li> <li>7. O.R. Rodig, C.E. Bell Jr. and A.K. Clark, Organic Chemistry Laboratory Standard and Microscale Experiments, Saunders College Publishing, 3<sup>rd</sup>edition, 2009.</li> <li>8. J. Mohan, Organic Analytical Chemistry, Narosa Publishing House, 2014.</li> </ol>	
<b>Course outcomes</b>	<ol style="list-style-type: none"> <li>1. Students will be in a position to understand stoichiometric requirements during organic syntheses.</li> <li>2. Students will be in a position to understand Safe and good laboratory practices, handling laboratory glassware, equipment and chemical reagents.</li> <li>3. Students will be in a position to apply the practical knowledge to perform experiments involving common laboratory techniques like reflux, distillation, steam distillation, vacuum distillation, aqueous extraction, thin layer chromatography (TLC) etc.</li> <li>4. Students will get hands-on experience on isolation of some important natural products.</li> </ol>	

Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHO-522

Title of the course: Practical Course in Organic Chemistry-II

Number of Credits: 02

Effective from AY: 2022-23

<b>Prerequisites for the course</b>	Students should have studied chemistry practical courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
<b>Course Objective:</b>	To translate certain theoretical concepts learnt earlier into experimental knowledge by providing hands on experience of basic laboratory techniques required for organic syntheses.	
<b>Content</b>	<i>Minimum 13 experiments from the list shall be conducted.</i> <b>1. Introduction to laboratory equipments, apparatus and safety</b> a. Common Hazards in Chemical Laboratory, Risk assessment b. Accidents and Emergency procedures	No of hours 04
	<b>2. Laboratory Techniques (Any Two)</b> a. Simple distillation i. Simple distillation of thionyl chloride under anhydrous condition ii. Simple distillation under Nitrogen atmosphere b. Fractional distillation i. Chloroform-dichloromethane mixture using water condenser. ii. Toluene and cyclohexane by fractionating column. c. Vacuum distillation under inert atmosphere Dry Distillation of DMF, <i>o</i> -dichlorobenzene, POCl <sub>3</sub> d. Thin layer Chromatography i. Purification and isolation of mixture of acids by using Preparative TLC. ii. Purification and isolation of mixture of phenols by using Preparative TLC. iii. Purification and isolation of pharmaceutical drugs using Preparative TLC.	08
	<b>3. Organic Synthesis (Any Four)</b> a. <i>p</i> -Iodonitrobenzene by Sandmeyer reaction b. Pinacol- Pinacolone rearrangement c. Hydrogenation of Maleic acid (Hydrogen balloon) d. Preparation of nitrostyrene from aldehyde e. Preparation of $\alpha,\beta$ -dibromocinnamic acid f. Reduction of nitro compounds g. Synthesis of Urea from ammonium cyanate	16

	<p><b>4. Solvent Free Organic synthesis (Any Two)</b></p> <p>a. Reduction using ball milling technique</p> <p>b. Oxidation of 2° alcohol using KMnO<sub>4</sub>/Alumina by grinding technique.</p> <p>c. Synthesis of (±)-Binol from β-naphthol</p> <p>d. Hunsdiecker reaction of cinnamic acid derivatives</p> <p>e. Beckmann rearrangement of oxime derivatives</p>	08
	<p><b>5. Two-step Organic Synthesis (Any Two)</b></p> <p>a. Benzamide-Benzoic acid-Ethyl Benzoate</p> <p>b. Phthalic anhydride – Phthalimide – Anthranilic acid.</p> <p>c. Methyl benzoate- <i>m</i>-nitrobenzoate- <i>m</i>-nitrobenzoic acid</p> <p>d. Chlorobenzene – 2, 4 – dinitrochlorobenzene – 2,4-dinitrophenol</p> <p>e. Acetanilide – <i>p</i>-Bromo acetanilide – <i>p</i>-Bromoaniline</p> <p>f. Acetophenone – Oxime – Acetanilide</p>	16
	<p><b>6. Separation, Isolation and Identification of Organic compounds (Any One)</b></p> <p>a. Separation, purification and identification of compounds of binary mixture (Solid-Solid, Solid-liquid and Liquid-liquid) using the TLC and column chromatography, chemical tests. IR spectra to be used for functional group identification.</p>	08
<b>Pedagogy</b>	Students should be given suitable pre- and post-lab assignments and explanation revising the theoretical aspects of laboratory experiments prior to the conduct of each experiment.	
<b>References / Readings</b>	<p>1. A. I. Vogel, A. R. Tatchell, B. S. Furniss, A. J. Hannaford, Vogel's Textbook of Practical Organic Chemistry, 5<sup>th</sup> Ed., Prentice Hall; 2011.</p> <p>2. K. Tanaka, Solvent-free Organic Synthesis, Wiley-VCH, 2<sup>nd</sup> Ed., 2009</p> <p>3. L. F. Fieser, K. L. Williamson "Organic Experiments" 7<sup>th</sup> edition D. C. Heath, 1992.</p> <p>4. K. L. Williamson, K. M. Masters, Macroscale and Microscale Organic Experiments, 6<sup>th</sup> Edition, Cengage Learning, 2010</p> <p>5. R. K. Bansal, Laboratory Manual in Organic Chemistry, New Age International, 5<sup>th</sup> Edition, 2016.</p> <p>6. S. Delvin, Green Chemistry, Sarup &amp; Sons, 2005.</p> <p>7. O. R. Rodig, C. E. Bell Jr., A. K. Clark, Organic Chemistry Laboratory Standard and Microscale Experiments, Saunders College Publishing, 3<sup>rd</sup> edition, 2009.</p> <p>8. J. Mohan, Organic Analytical Chemistry, Narosa Publishing House, 2014.</p>	
<b>Course outcomes</b>	<p>1. Students will be in a position to adopt Safe and good laboratory practices, handling laboratory glassware, equipment and chemical reagents.</p> <p>2. Students will be in a position to understand and calculate stoichiometric requirements during organic syntheses.</p>	

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|  | <ol style="list-style-type: none"><li>3. Students will be in a position to perform common laboratory techniques including reflux, distillation, vacuum distillation, aqueous extraction, thin layer chromatography (TLC).</li><li>4. Students will get hands-on experience on isolation of some important natural products.</li></ol> |
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Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHP-500 Title of the course: General Physical Chemistry

Number of Credits: 04

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied chemistry courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
<b>Course Objective:</b>	1. Introduction of various concepts on thermodynamics. 2. Introduction of electro chemistry and kinetics. 3. Learning quantum chemistry.	
<b>Content</b>	<b>1. Mathematical Preparations</b> a. Introduction to various functions and function plotting (exponential, logarithmic, trigonometric etc.), functions of many variables. Complex numbers and complex functions. b. Linear equations, vectors, matrices and determinants. c. Basic rules of differentiation and integration, Partial differentiation, location and characterization of critical points of a function, Regression methods, curve fitting. d. Introduction to series, convergence and divergence, power series, Fourier series e. Probability (permutations and combinations).	No of hours  12
	<b>2. Quantum Chemistry</b> a. Operators, Functions, Eigen value equations, Postulates. b. Schrodinger equation, application to simple system viz. free particle, particle in one dimensional, two dimensional and three-dimensional box (quantization, separation of variables, degenerate wave functions). c. Hydrogen like atoms, Schrodinger equation and its solutions, atomic orbital wave functions and interpretation. d. Hückel MO theory, Secular equations, Secular determinant, delocalization energy, charge density, $\pi$ -bond order, free valence, applications to $C_2H_4$ , $C_3H_5$ (radical), $C_4H_6$ , $C_4H_4$ , $C_6H_6$ , $C_6H_8$ .	20
	<b>3. Thermodynamics</b> a. Thermodynamic properties: Gas laws, Real gasses, Boyle temperature, Critical temperature, State and path properties. Intensive and extensive properties. Exact and inexact differentials. Internal energy, enthalpy, entropy, free energy and their relations and significances. Maxwell relations. Thermodynamic equations of state b. Joule-Thomson effect. Joule-Thomson coefficient for van der	12

	<p>Waals' gas. Joule-Thomson effect and production of low temperature, adiabatic demagnetization, Joule-Thomson coefficient, inversion temperature.</p> <p>c. The third law of thermodynamics. Need for the third law. Apparent exceptions to third law. Application of third law. Use of thermodynamic functions in predicting direction of chemical change. Entropy and third law of thermodynamics.</p> <p>d. Phase equilibria: Phase rule, Discussion of two component systems forming solid solutions with and without maximum or minimum in freezing point curve. Systems with partially miscible solid phases.</p> <p>e. Three component systems: Graphical representation. Three component liquid systems with one pair of partially miscible liquids. Influence of temperature. Systems with two pairs and three pairs of partially miscible liquids. The role of added salts.</p>	
	<p><b>4. Electrochemistry</b></p> <p>a. EMF series, The cell potential: The Nernst equation, Cells at equilibrium. Determination of thermodynamic functions.</p> <p>b. Decomposition potential and overvoltage, electronegativity, basic principles, completeness of deposition, Separation with controlled potentials, constant current electrolysis, composition of electrolyte, potential buffers, physical characteristics of metal deposits.</p> <p>c. Electroplating and electroless plating, electrosynthesis.</p> <p>d. Concepts of acid-base aqueous and non-aqueous solvents, hard and soft acid-base concept and applications.</p>	8
	<p><b>5. Chemical Kinetics</b></p> <p>a. General introduction to various types of order of reaction including fractional order, Molecularity of the reaction.</p> <p>b. Introduction to reversible and irreversible reactions and reactions leading to equilibrium. Van't Hoffs equation and analysis of Gibbs free energy of equilibrium reactions.</p> <p>c. Collision Theory and Maxwell Boltzmann distribution of energies of colliding molecules (derivation not required). The concept of collisional cross section and reactive cross section and its significance.</p> <p>d. Comparative study of transition state and collision state theory (derivation not required).</p> <p>e. Reaction Mechanisms: elementary reactions, Consecutive elementary reactions, steady state approximation, the rate determining step and pre-equilibria</p> <p>f. Free radical reactions, Complex reactions such as acetaldehyde decomposition and reaction between H<sub>2</sub> and Br<sub>2</sub>, Homogeneous reactions and acid-base catalysis.</p>	8

	g. Elementary enzyme reactions. Lineweaver-Burk plot and its analysis	
<b>Pedagogy</b>	Mainly lectures and tutorials. Seminars / term papers / assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
<b>References / Readings</b>	<ol style="list-style-type: none"> <li>1. P. W. Atkins and J. D. Paula, Physical Chemistry, 8<sup>th</sup> Ed., Oxford University Press, New Delhi. 2007</li> <li>2. G. M. Barrow, Physical Chemistry, 5<sup>th</sup> Ed., Tata McGraw Hill, New Delhi. 2016</li> <li>3. J. E. House, Principles of Chemical Kinetics, 2<sup>nd</sup> Ed., Academic Press, Elsevier Burlington, USA, 2007</li> <li>4. I. N. Levine, Quantum Chemistry, 7<sup>th</sup> Ed., Prentice-Hall, New Delhi. 1999</li> </ol>	
<b>Course outcomes:</b>	<ol style="list-style-type: none"> <li>1. Students should be in a position to understand and explain various concepts in physical chemistry.</li> <li>2. Students should be in a position to apply these concepts during the lab course in physical chemistry.</li> <li>3. Students will understand concepts of electrochemistry.</li> <li>4. Students will be able to apply fundamentals of chemical kinetics for understanding reaction mechanisms.</li> </ol>	

**Name of the Programme:** M.Sc. Part-I (Chemistry)

**Course Code:** CHP-521      **Title of the course:** Practical course in Physical Chemistry-I

**Number of Credits:** 02

**Effective from AY:** 2022-23

<b>Prerequisites for the course:</b>	Students should have studied chemistry courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
<b>Course Objective:</b>	1. To develop experimental skills on basic lab techniques in physical chemistry 2. To acquire skills for data analysis and interpretation 3. To help the students to develop research skills	
<b>Content</b>	Minimum 13 Experiments to be performed per Semester Non-instrumental Experiments (any 7)  1. To study the kinetics of hydrolysis of ethyl acetate and to determine a) Energy of activation b) Entropy of activation and c) Free energy change. 2. To determine the order of reaction between potassium persulphate and potassium iodide by graphical, fractional change and differential methods. 3. To study the three-component system such as acetic acid, chloroform; and water and obtain tie line. 4. To determine the molecular weight of polyvinyl alcohol by viscosity measurement. 5. To study the electro-kinetics of rapid reaction between $\text{SO}_4^{2-}$ and $\text{I}^-$ in an aqueous solution. 6. To determine the buffer capacity of acidic buffer solution. 7. To determine the partial molal volume of ethanol-water mixture at a given temperature. 8. To measure energy content of various types of plastics using bomb calorimetry 9. To determine number average molecular weight of a polymer sample with an indirect titration method. 10. To investigate basic hydrolysis of ethyl acetate at four different temperatures and find out energy of activation	No of hours  30
	Instrumental Experiments (any 6)	



	<p>11. To determine the degree of hydrolysis of salt of weak base and strong acid using conductometer.</p> <p>12. To determine the dissociation constants of a tribasic acid (Phosphoric acid obtain derivative plot to get equivalence point.</p> <p>13. To determine formal redox potential of <math>\text{Fe}^{2+}/\text{Fe}^{3+}</math> and <math>\text{Ce}^{3+}/\text{Ce}^{4+}</math> system obtain derivative plot to get equivalence point.</p> <p>14. To study spectrophotometric titration of ferrous ammonium sulphate with potassium permanganate (or dichromate vs permanganate)</p> <p>15. To determine Avogadro's number by improved electroplating.</p> <p>16. To determine the zeta potential of colloidal system and investigate the effect of different surfactants on stability of the colloids</p> <p>17. To verify the Kohlrausch's law for weak electrolyte by conductometry</p> <p>18. To determine the transport numbers of <math>\text{Cu}^{2+}</math> and <math>\text{SO}_4^{2-}</math> ions in <math>\text{CuSO}_4</math> solution by Hittorf's method.</p>	30
<b>Pedagogy</b>	Mainly pre-laboratory exercises Seminars / term papers / assignments / presentations / lab hand-out / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
<b>References / Readings</b>	<ol style="list-style-type: none"> <li>1. A. Finlay &amp; J.A. Kitchener, Practical Physical Chemistry, Longman.</li> <li>2. F. Daniels &amp; J.H. Mathews, Experimental Physical Chemistry, Longman.</li> <li>3. A. M. James, Practical Physical Chemistry, Longman.</li> <li>4. D.P. Shoemaker &amp; C.W. Garland, Experimental Physical Chemistry, McGraw-Hill.</li> </ol>	
<b>Course outcomes:</b>	<ol style="list-style-type: none"> <li>1. Students will able to explain various fundamental lab techniques.</li> <li>2. Students should be in a position to apply the knowledge for their dissertation and research work.</li> <li>3. Students will be able to use spectrophotometric titrations for appropriate analysis.</li> <li>4. Students will be able to determine molecular weight of some polymers.</li> </ol>	

Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHP-522 Title of the course: Practical course in Physical Chemistry-II

Number of Credits: 02

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied chemistry courses at graduate level or must have cleared change of discipline entrance test.	
<b>Course Objective:</b>	1. To develop experimental skills on basic lab techniques in physical chemistry 2. To acquire skills for data analysis and interpretation 3. To help the students to develop research skills	
<b>Content</b>	<p>Minimum 13 experiments to be conducted per Semester</p> <p><b>Non-instrumental Experiments (any 8)</b></p> <ol style="list-style-type: none"><li>1. To determine the radius of a molecule by viscosity measurements.</li><li>2. To determine <math>\Delta G</math>, <math>\Delta H</math> and <math>\Delta S</math> of silver benzoate by solubility product method</li><li>3. To investigate the adsorption of oxalic acid by activated charcoal and test the validity of Freundlich and Langmuir's isotherms.</li><li>4. To determine the molecular weight of a given polymer by turbidimetry</li><li>5. To study the rate of reaction between ethyl bromoacetate and sodium thiosulphate kinetically.</li><li>6. To determine the percentage composition of a given mixture of two liquids by stalagmometer method.</li><li>7. To study the kinetics of hydrolysis of methyl acetate and to determine a) Energy of activation b) Entropy of activation and c) Free energy change.</li><li>8. To study the kinetics of the reaction between Potassium persulphate (<math>K_2S_2O_8</math>), and Potassium iodide (KI), and to determine a) Energy of activation b) Entropy of activation and c) Free energy change.</li><li>9. To determine the order of reaction for hydrolysis of ethyl acetate by graphical, fractional change and differential methods.</li><li>10. To determine the molecular weight of polystyrene by</li></ol>	No of hours 35

	viscosity measurement.	
	<p><b>Instrumental Experiments (any 5)</b></p> <p>11. To determine the relative strength of chloroacetic acid and acetic acid by conductometry.</p> <p>12. To determine the degree of hydrolysis of salt of weak base and strong acid using conductometry.</p> <p>13. To determine the composition of a mixture of acetic acid, dichloroacetic acid and hydrochloric acid by conductometric titration.</p> <p>14. To determine the dissociation constants of monobasic acid and dibasic acid and obtain derivative plot to get equivalence point.</p> <p>15. To determine the redox potential of <math>\text{Fe}^{2+}/\text{Fe}^{3+}</math> system by titrating it with standard <math>\text{K}_2\text{Cr}_2\text{O}_7</math> solution.</p> <p>16. To study the electrodeposition of metal.</p>	25
<b>Pedagogy</b>	Mainly pre-laboratory exercises Seminars / term papers /assignments / presentations / lab hand-out /self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
<b>References / Readings</b>	<ol style="list-style-type: none"> <li>1. A. Finlay &amp; J.A. Kitchener, Practical Physical Chemistry, Longman.</li> <li>2. F. Daniels &amp; J.H. Mathews, Experimental Physical Chemistry, Longman.</li> <li>3. A. M. James, F. E. Prichard, Practical Physical Chemistry, Longman.</li> <li>4. D.P. Shoemaker &amp; C.W. Garland, Experimental Physical Chemistry, McGraw-Hill.</li> </ol>	
<b>Course outcomes:</b>	<ol style="list-style-type: none"> <li>1. Students will gain knowledge of various fundamental lab techniques.</li> <li>2. Students should be in a position to apply the knowledge for their dissertation and research work.</li> <li>3. Students will be able to use spectrophotometric titrations for appropriate analysis.</li> <li>4. Students will be able to determine molecular weight of some polymers.</li> </ol>	

Name of the Programme: M. Sc -I (Physical Chemistry)

Course Code: CHP-501      Title of the course: Quantum Chemistry and Statistical Thermodynamics

Number of Credits: 04

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied physical chemistry courses at M.Sc. Chemistry in semester I	
<b>Course Objective:</b>	1. Introduction of various concepts of quantum chemistry. 2. To introduce various concepts of statistical thermodynamics.	
<b>Content</b>	<b>1. Quantum Chemistry</b> a. The origin of quantum mechanics: Planck's quantum theory, wave particle duality, uncertainty principle concept of wave function, the Born interpretation of wave function. Normalization and orthogonalizations, quantization, Eigen values and Eigen functions. b. Postulates of quantum mechanics; Schrödinger equation for free particle, particle in a box, degeneracy. Quantum mechanical operators and their properties, commutation relations, Hamiltonian and Laplacian operators, Harmonic oscillators, Angular momentum, Ladder Operators. c. Approximate methods, Schrödinger equation, its importance and limitations, Born-Oppenheimer approximation, Anti-symmetric wave functions and Slater determinants (many electron system e.g. He atom), Exclusion and Aufbau principle, Variation method, Linear Variation Principle, Perturbation theory (first order non-degenerate) and their applications to simple systems. d. MO theory, Hückel MO theory, Bond-order, Charge density matrix, Unification of HMO and VB theory, their applications in spectroscopy and chemical reactivity, electron density forces and their role in chemical bonding. Hybridization and valence MOs of H <sub>2</sub> O, NH <sub>3</sub> and CH <sub>4</sub> . Application of Hückel Theory to ethylene, butadiene and benzene molecules.	No of hours  34
	<b>2. Statistical Thermodynamics</b> a. The language of statistical thermodynamics: Probability, ensemble, microstate, degeneracy, permutations and combinations. Configuration and weights, the dominant configuration. The Boltzmann distribution. The molecular partition function: its interpretation and its relation to	26

	<p>uniform energy levels.</p> <p>b. Translational, Rotational, Vibrational and Electronic Partition functions for diatomic molecules. Relation between thermodynamic functions and partition functions and their statistical interpretations. Equilibrium constants from partition function.</p> <p>c. Law of Equipartition energy. Theories of specific heat of solids. Comparison between Einstein and Debye theories.</p> <p>d. Concept of symmetric and antisymmetric wave functions. Ortho and para hydrogens. Quantum Statistics: Fermi-Dirac (FD) and Bose-Einstein (BE) statistics. Comparison between MB, FD and BE Statistics.</p>	
<b>Pedagogy</b>	<p>Mainly lectures and tutorials. Seminars / term papers / assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.</p>	
<b>References / Readings</b>	<ol style="list-style-type: none"> <li>1. P. W. Atkins and J. D. Paula, Physical Chemistry, 8<sup>th</sup> Ed., Oxford University Press, New Delhi. 2007</li> <li>2. G. M. Barrow, Physical Chemistry, 5<sup>th</sup> Ed., Tata McGraw Hill, New Delhi. 2016.</li> <li>3. M.C. Gupta, Statistical Thermodynamics, Wiley Eastern, New Delhi. 1990</li> <li>4. I. N. Levine, Quantum Chemistry, 7<sup>th</sup> Ed., Prentice-Hall, New Delhi. 1999</li> <li>5. H. Metiu, Physical Chemistry, Statistical Mechanics, Taylor &amp; Francis, New York, 2006</li> </ol>	
<b>Course outcomes:</b>	<ol style="list-style-type: none"> <li>1. Students should be in a position to understand and explain various concepts of quantum chemistry viz. the wave function and applications.</li> <li>2. Students should be able to explain various concepts in statistical thermodynamics viz. the partition function and applications.</li> <li>3. Students will be able to explain postulates of quantum mechanics.</li> <li>4. Students will be able to explain law of equipartition energy.</li> </ol>	

Name of the Programme: M. Sc -I (Physical Chemistry)

Course Code: CHP-502 Title of the course: Group Theory and Molecular Spectroscopy

Number of Credits: 04

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied physical chemistry courses at M.Sc. Chemistry in semester I	
<b>Course Objective:</b>	1. To introduce concepts in Group Theory and its applications to chemistry. 2. To introduce some advanced topics in spectroscopy.	
<b>Content</b>	<b>1. Group Theory for Chemistry</b> a. Symmetry elements and symmetry operations, Concept of group and group multiplication tables, order of the group, classes and subgroups in a group, Different types of groups (cyclic, abelian and non-abelian groups). b. Point groups, Matrix representations of a group, Reducible and Irreducible representations groups, Great Orthogonality Theorem, Properties of Irreducible representations, Mulliken symbols for Irreducible representations, Character tables. c. Standard reduction formula, Direct products of representations and its applications Quantum Chemistry and spectroscopy: Vanishing of integrals, Selection rules. Applications of group theory for hybridization of atomic orbitals. Projection operator and Symmetry adapted linear combinations (SALCs), MO treatment (within Huckel Molecular Orbital Theory) of large molecules with symmetry. Applications of group theory to Infra-red and Raman spectroscopy. d. Space Groups: Symmetry elements, Schoenflies, and Hermann Mauguin notation, Representation of point groups and space groups, point symmetry, space symmetry, glide plane, helical screw axis	No of hours  30
	<b>2. Microwave, IR and Raman Spectroscopy</b> a. Theoretical treatment of Rotational and Vibrational spectroscopy. b. Principle of Fourier Transform (FT) spectroscopy, FTIR spectroscopy: Theory, instrumentation and applications. c. Quantum theory of Raman effect, Raman shift, Instrumentation, Resonance Raman spectroscopy, Complimentary nature of IR and Raman spectroscopy in	12

	structure determination, Applications.	
	<b>3. NMR Spectroscopy</b> a. Basic principles of NMR b. Theory of pulse NMR and Fourier analysis, FT-NMR. c. Solid state NMR, magic angle spinning (MAS), dipolar decoupling and cross polarization, applications of solid-state NMR. d. Double resonance, NOE, Spin tickling, Solvent and shift reagents, Structure determination by NMR.	10
	<b>4. ESR Spectroscopy</b> a. Theory and experimental techniques, Identification of odd-electron species (methyl and ethyl free radicals) and radicals containing hetero atoms. b. Spin trapping and isotopic substitution, Spin densities and McConnell relationship, Double resonance techniques.	8
<b>Pedagogy</b>	Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
<b>References / Readings</b>	1. P. W. Atkins and J. D. Paula, Physical Chemistry, 8 <sup>th</sup> Ed., Oxford University Press, New Delhi, 2007. 2. F.A. Cotton, Chemical Applications of Group Theory, 3 <sup>rd</sup> Ed., John Wiley & Sons-Asia, New Delhi, 1999 3. K. V. Raman, Group Theory and its applications to chemistry, Tata McGraw-Hill, New Delhi, 1999 4. C. N. Banwell and E.M. McCash, Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill, New Delhi, 1994 5. W. Kemp, NMR in Chemistry a multinuclear introduction, Macmillan, 1986. 6. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders Company, 1977.	
<b>Course outcomes:</b>	1. Students should be in a position to explain various concepts in Group Theory. 2. Should be able to apply character table to solve various problems. 3. Students should be in a position to apply the knowledge of spectroscopy for their dissertation and research work. 4. Students will understand the fundamental difference between various spectroscopic techniques.	

Name of the Programme: M. Sc -I (Physical Chemistry)

Course Code: CHP-503 Title of the course: Chemical Kinetics and Thermodynamics

Number of Credits: 04

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied physical chemistry courses at M.Sc. Chemistry in semester I	
<b>Course Objective:</b>	1. To introduce concepts of reaction kinetics and thermodynamics 2. To provide fundamental knowledge of theories that govern chemical reactions 3. To introduce newer classes of reaction types and their kinetics 4. To introduce latest developments in the advance instrumental techniques and methods for monitoring reaction kinetics and dynamics.	
<b>Content</b>	<b>1. Theories of reaction rates</b> a. Generalized kinetic theory and extended collision theory. Concept of collisional number, collisional frequency factor, collisional and reactive cross section, steric factor, microscopic rate constant. Assumptions and limitations of collision theory. b. Conventional transition state theory, equilibrium hypothesis and derivation of reaction rates. Thermodynamic formulation of transition state theory. Arrhenius temperature dependent and independent activation energy and its significance. Assumptions and limitations of transition state theory. Lindemann-Hinshelwood theory of thermal unimolecular reactions.	No of hours 10
	<b>2. Elementary reactions in solutions</b> Collisional kinetics in solution, effect of solvent polarity, solvent cohesion energy, and ion-dipole and dipole-dipole reactions on reaction rates.	3
	<b>3. Kinetics of Homogeneous reactions</b> Homogeneous kinetics, enzymatic reactions and Michaelis-Menten, Lineweaver-Burk and Eadie Analysis, Autocatalytic reactions.	5
	<b>4. Composite reactions</b> Types of composite mechanisms, kinetics of parallel and consecutive reactions. Introduction to shock tube method and its use in combustion analysis.	3
	<b>5. Fast Reactions</b> Photochemical fast reactions, Pulsed laser photolysis, and its use in monitoring fast reactions.	3
	<b>6. Reversible, Irreversible and Oscillatory reactions.</b>	4



	<p>a. Kinetics of reversible reactions and graphical analysis</p> <p>b. Oscillatory reactions, Voltera-Lotka hypothesis of oscillatory reactions. The significance of bi-stability in the Briggs-Rauscher Reaction and Belousov-Zhabotinskii reaction.</p>	
	<p><b>7. Reaction Dynamics</b></p> <p>Introduction to potential energy surfaces, description of H<sub>2</sub>O and HF potential energy surface diagrams.</p>	2
	<p><b>8. Equilibrium Thermodynamics</b></p> <p>a. Important terminologies in Thermodynamics; Thermodynamics state functions; work &amp; heat; work expansion; Mathematical interlude Exact and inexact differentials. Cyclic rule; partial derivatives.</p> <p>b. Heat change at constant pressure, volume; relationship between Q<sub>p</sub> &amp; Q<sub>v</sub>; Heat capacities C<sub>p</sub>, C<sub>v</sub>; Concept of Entropy, entropy change for an ideal gas at different conditions; Entropy of mixing of ideal gas and the Gibbs paradox; Physical significance of entropy.</p> <p>c. Work function and free energy function; Variation of free energy with temperature and pressure; Maxwell relations; Thermodynamic equations of state; Gibbs-Helmholtz equation.</p> <p>d. Thermodynamics of open systems, partial molar properties; chemical potential, variation of chemical potential with temperature and pressure; Gibbs-Duhem equation; Duhem-Margules equation; applications of chemical potential; thermodynamic derivation of phase rule.</p>	17
	<p><b>9. Non-Equilibrium thermodynamics</b></p> <p>a. Concept of internal entropy and spontaneity of a process in relation to free energy. Chemical affinity and extent of a reaction. Phenomenological Laws and Onsager's Reciprocal Relations; Conservation of Mass and energy in closed and open system.</p> <p>b. Postulates of non-equilibrium thermodynamics. Entropy production in heat flow. Entropy production of chemical reactions and Entropy production/entropy flow in open system.</p> <p>c. Principle of microscopic reversibility and the Onsager reciprocal relations; Validity of Onsager's equation and its verification; Application of Irreversible Thermodynamics to Biological Systems; Application to thermo-electric and electrokinetic phenomena.</p>	13
<b>Pedagogy</b>	<p>Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.</p>	
<b>References /</b>	<p>1. K. J. Laidler, Chemical Kinetics, 3<sup>rd</sup> Ed.; Pearson Education, 1987;</p>	

<p><b>Readings</b></p>	<p>(printed in India by Anand Sons, 2004).</p> <ol style="list-style-type: none"> <li>2. P.W. Atkins and J. De. Paulo, Atkins' Physical Chemistry, 8<sup>th</sup> Ed. Oxford University Press, 2007.</li> <li>3. J. I. Steinfeld, J. S. Francisco and W. L. Hase, Chemical Kinetics and Dynamics, 2<sup>nd</sup> Ed.; Prentice Hall, 1999.</li> <li>4. D. K. Chakrabarty and B. Viswanathan, Heterogeneous Catalysis, New Age International Publishers, 2008.</li> <li>5. S. K. Scott, Oscillations, waves and Chaos in chemical kinetics, Oxford Science Publications, 1994.</li> <li>6. T. S. Briggs, and W. C. Rauscher, An oscillating iodine clock, J. Chem. Educ., 1973.</li> <li>7. G. W. Castellan, Physical Chemistry, 3<sup>rd</sup> Ed.; University of Maryland, Addison-Wesley Publishing Company, 1983.</li> <li>8. E. N. Yeregin, Fundamentals of Chemical Thermodynamics Firebird Publications, 1978.</li> <li>9. D. A. McQuarrie &amp; John D. Simon, Physical Chemistry: A molecular approach, Viva Books Pvt. Ltd., New Delhi, 2019.</li> <li>10. S. R. De Groot, Non-equilibrium thermodynamics, Dover Publications, 2011.</li> <li>11. A. Kleidon, R.D. Lorenz (Eds.), Non-equilibrium thermodynamics and the production of entropy: life, earth, and beyond, Springer Berlin Heidelberg New York, 2005.</li> <li>12. J. Rajaram, J. C. Kuriacose, S. N. &amp; Co., Thermodynamics for students of Chemistry, Classical, Statistical and Irreversible, Jalandhar, 1996.</li> <li>13. P. W. Atkins &amp; J. De. Paulo, Atkins' Physical Chemistry, 8<sup>th</sup> Ed.; Oxford Univ. Press, 2007.</li> </ol>
<p><b>Course outcomes:</b></p>	<ol style="list-style-type: none"> <li>1. Students should be in a position to understand and explain various concepts in chemical kinetics and thermodynamics.</li> <li>2. Students should be in a position to apply these concepts during the lab course in experimental physical chemistry.</li> <li>3. Students will able to explain the concept of equilibrium and non-equilibrium thermodynamics.</li> <li>4. Students will able to explain the elementary reactions in solutions.</li> </ol>

Name of the Programme: M. Sc -I (Physical Chemistry)

Course Code: CHP-504      Title of the course: Electrochemistry and Surface Studies

Number of Credits: 04

Effective from AY: 2022-23

<b>Prerequisites for the course:</b>	Students should have studied physical chemistry courses at M.Sc. Chemistry in semester I	
<b>Course Objective:</b>	1. To introduce some core concepts of electrochemical processes including ionic interaction theories, electrified interfaces, electrochemical kinetics and thermodynamics 2. To develop problem solving skills in electrochemistry 3. To introduce fundamental concepts and applications of electrochemistry in day-today life eg. batteries, solar cells, capacitors	
<b>Content</b>	<b>1. Ionic Interactions and Conductance in Electrolytes</b> a. Ion-solvent interactions. Born Theory, validity and limitations. b. Solvation number and coordination number. c. Ion-ion interactions and Debye-Huckel theory of ion cloud. d. Applications of Debye- Huckel equation. Concept of ionic strength and activity coefficient. e. Debye-Huckel limiting law and its modifications. f. Debye-Huckel-Onsager equation, validity and limitations. g. Einstein-Smoluchowski equation. h. Influence of ionic atmospheres on ionic migration: Relaxation and Electrophoretic effects. i. Conductance in strong and weak electrolytes.	No of hours  10
	<b>2. Electrified Interfaces</b> a. Formation of an electrode/electrolyte interface and its structure. b. Polarizable and non-polarizable interfaces. c. Potential difference across electrical double layer: outer potential, surface potential, inner potential and relationship between them, chemical and electrochemical potentials. d. Thermodynamics of electrified interface: Surface tension, surface excess, Electro-capillary curves. Determination of surface excess. Condition for thermodynamic equilibrium at electrified interface. e. Generalized Gibbs equation, Lippmann equation and electrical capacitance at the double layer. f. Models of the electrified interface. g. Ion adsorption at the electrode: hydrated electrodes, contact adsorption,	10

	Gibbs adsorption equation.	
	<b>3. Pure Liquid Electrolytes: Ionic Liquids</b> a. Thermal loosening of ionic lattice. b. Ionic liquids in surface electrochemistry: Electrode/electrolyte interfacial processes in ionic liquids. c. Electrochemistry of Ti (IV) in Ionic liquids.	8
	<b>4. Electrode Kinetics and Corrosion</b> a. Disturbance of electrode equilibrium, cause of electron transfer, fast and slow systems and their current-potential relationship. b. Butler-Volmer equation and its low and high field approximations. c. Nernst equation as a special case of B-V equation. d. Tafel plots for anodic and cathodic processes. e. Fundamentals of Impedance spectroscopy; determining exchange current densities and rate constants from impedance plots. f. Principles of corrosion, electrochemical methods of avoiding corrosion. g. pH-potential diagrams: Pourbaix diagram for corrosion of iron and stability of water.	12
	<b>5. Colloidal Chemistry</b> a. Interaction of double layers and stability of Sols. DLVO theory. b. Colloidal electrolytes, critical micelle concentration, Kraft temperature. c. Electrokinetic phenomena: Electroosmosis, streaming potential and current, electrophoresis. Zeta potential. d. Donnan membrane equilibria. e. Micelles and reverse micelles, Emulsions and Microemulsions.	8
	<b>6. Electrochemical Energies: Conversion and Storage</b> a. Thermodynamics of electrochemical energy conversion. b. Batteries: Basic principles; rating and shelf life. Zinc-Manganese dioxide: Leclanche and alkaline batteries. Lithium ion batteries and recharge ability. c. Fuel cells: Principle of a hydrogen-oxygen fuel cell. Classification of fuel cell systems based on types of electrolytes/temperature. Efficiency w.r.t. thermodynamic efficiency, reliability and economic benefits. Direct methanol-polymer electrolyte fuel cell and electro-catalysts - a case study. Reactions occurring in various fuel cells and calculation of their electrode and cell potentials. d. Super-capacitors: Introduction: Origin of Supercapacitance.	7
	<b>7. Photoelectrochemistry</b>	5

	<p>a. Semiconductor/Electrolyte Interface: Band edge and Band bending.</p> <p>b. Light absorption and carrier generation at the electrode: photoinduced charge transfer, hot carriers.</p> <p>c. Photoelectrodes: p-type photocathode, n-type photoanode.</p> <p>d. Determination of surface states.</p> <p>e. Photoelectrocatalysis: photoelectrochemical water splitting and CO<sub>2</sub> reduction.</p> <p>f. Types of photoelectrochemical devices.</p>	
<b>Pedagogy</b>	Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
<b>References / Readings</b>	<ol style="list-style-type: none"> <li>1. J. O. M. Bockris &amp; A. K. N. Reddy, Modern Electrochemistry, Springer India, Pvt.Ltd, 2000, Vol.1,2and3.</li> <li>2. D. Crow, Principles and Applications of Electrochemistry, Blackie Academy and Professional, 1994.</li> <li>3. C. M. A. Brett &amp; A. M. O. Brett, Electrochemistry: Principles, methods and applications, Oxford, NewYork Oxford University Press, 1993.</li> <li>4. R. D. Vold &amp; M. J. Vold, Colloid and Interface Chemistry, Addison-Wesley, 1983.</li> <li>5. A. Vincent &amp; B. Sacrosati, Modern Batteries, John Wiley, NewYork,1997.</li> <li>6. J. O. M. Bockris &amp; S. Srinivasan, Fuelcells: Their Electrochemistry, McGraw-HillBook Co., 1969.</li> <li>7. A. A. J. Torriero, Electrochemistry in Ionic Liquids, Vol. 1: Fundamentals, Springer International Publishing, 2015</li> <li>8. B. A.J., Stratmann M., Licht D, Encyclopedia of Electrochemistry, Semiconductor Electrodes and Photoelectrochemistry, Wiley-VCH, 2002.</li> </ol>	
<b>Course outcomes:</b>	<ol style="list-style-type: none"> <li>1. Students will be in a position to explain various fundamental and core concepts of electrochemistry.</li> <li>2. Students should be in a position to apply the knowledge of electrochemistry for their dissertation and research work</li> <li>3. Students should be in a position to apply these concepts during the lab course in physical chemistry</li> <li>4. Students will be able to explain the concepts of Photoelectrochemistry.</li> </ol>	

**M.Sc. Organic/Inorganic/Analytical/Physical Chemistry Part-II syllabus for AY 2023-24 (SEM III and SEM IV) based on NEP 2020**

<b>SEM III &amp; IV</b>			
<b>Research Specific Elective (RSE) Courses</b>			
<b>Sr. No.</b>	<b>Subject code</b>	<b>Paper title</b>	<b>Credits</b>
1.	<a href="#"><u>CHO-600</u></a>	Practical Course in Organic Chemistry-III	4
2.	<a href="#"><u>CHO-601</u></a>	Practical Course in Organic Chemistry-IV	4
3.	<a href="#"><u>CHO-602</u></a>	Retrosynthesis and Heterocyclic Chemistry	4
4.	<a href="#"><u>CHO-603</u></a>	Chemistry of Natural Products	4
5.	<a href="#"><u>CHI-600</u></a>	Practical Course in Inorganic Chemistry-III	4
6.	<a href="#"><u>CHI-601</u></a>	Practical Course in Inorganic Chemistry-IV	4
7.	<a href="#"><u>CHI-602</u></a>	Principles and applications in catalysis	4
8.	<a href="#"><u>CHI-603</u></a>	Selected Topics in Inorganic Chemistry	4
9.	<a href="#"><u>CHA-600</u></a>	Practical Course in Analytical Chemistry-III	4
10.	<a href="#"><u>CHA-601</u></a>	Practical Course in Analytical Chemistry-IV	4
11.	<a href="#"><u>CHA-602</u></a>	Advanced Mass Spectrometry	4
12.	<a href="#"><u>CHA-603</u></a>	Selected Topics in Analytical Chemistry	4
13.	<a href="#"><u>CHP-600</u></a>	Practical Course in Physical Chemistry-III	4
14.	<a href="#"><u>CHP-601</u></a>	Practical Course in Physical Chemistry-IV	4
15.	<a href="#"><u>CHP-602</u></a>	Heterogeneous Catalysis: Fundamentals and Applications	4
16.	<a href="#"><u>CHP-603</u></a>	Applied Electrochemistry	4
17.	<a href="#"><u>CHC-600</u></a>	Research Methodology and instrumental techniques-I	4
18.	<a href="#"><u>CHC-601</u></a>	Research Methodology and instrumental techniques-II	4
19.	<a href="#"><u>CHC-651</u></a>	Discipline Specific Dissertation	16
<b>Generic Elective (GE) Courses</b>			
<b>Sr. No.</b>	<b>Subject code</b>	<b>Paper title</b>	<b>Credits</b>
1.	<a href="#"><u>CHO-621</u></a>	Polymer Chemistry: Concepts, Synthesis and Processing of Polymers	4
2.	<a href="#"><u>CHO-622</u></a>	Concepts in Medicinal Chemistry	4
3.	<a href="#"><u>CHO-623</u></a>	Concepts in Green Chemistry	4
4.	<a href="#"><u>CHO-624</u></a>	Chemistry of Life	4
5.	<a href="#"><u>CHO-625</u></a>	Organometallic Chemistry and Rearrangement Reactions	4
6.	<a href="#"><u>CHI-621</u></a>	Bioinorganic Chemistry	4
7.	<a href="#"><u>CHI-622</u></a>	Chemistry of p-block elements & their compounds	4

8.	<a href="#"><u>CHI-623</u></a>	Environmental Chemistry	4
9.	<a href="#"><u>CHI-624</u></a>	Inorganic Chemistry: Industrial Perspective	4
10.	<a href="#"><u>CHA-621</u></a>	Fundamentals of Crystallography	4
11.	<a href="#"><u>CHA-622</u></a>	Advanced NMR and combined Spectroscopy	4
12.	<a href="#"><u>CHA-623</u></a>	Bioanalytical Techniques	4
13.	<a href="#"><u>CHA-624</u></a>	Calibration and Validation in Analytical Chemistry	4
14.	<a href="#"><u>CHP-621</u></a>	Solid State Chemistry: Concepts and Applications	4
15.	<a href="#"><u>CHP-622</u></a>	Nanoscience: Concepts and Applications	4
16.	<a href="#"><u>CHP-623</u></a>	Physical aspects of Polymer Chemistry	4
17.	<a href="#"><u>CHP-624</u></a>	Colloids and Surface Chemistry	4
		<b>Dissertation</b>	
1.	<a href="#"><u>CHC-651</u></a>	Discipline Specific Dissertation	16

**M.Sc. Physical Chemistry Part-II syllabus for AY 2023-24 (SEM III and SEM IV)**

<b>SEM III ORGANIC CHEMISTRY</b>			
<b>Sr. No.</b>	<b>Subject code</b>	<b>Paper title</b>	<b>Credits</b>
1	<b>CHP-600</b>	Practical Course in Physical Chemistry-III	4
2	<b>CHP-601</b>	Practical Course in Physical Chemistry-IV	4
3	<b>CHC-600</b>	Research Methodology and instrumental techniques-I	4
4	<b>CHC-601</b>	Research Methodology and instrumental techniques-II	4
5	<b>CHP-621</b>	Solid State Chemistry: Concepts and Applications	4
6	<b>CHP-622</b>	Nanoscience: Concepts and Applications	4
7	<b>CHP-623</b>	Physical aspects of Polymer Chemistry	4
8	<b>CHP-624</b>	Colloids and Surface Chemistry	4
<b>SEM-IV ORGANIC CHEMISTRY</b>			
1	<b>CHP-602</b>	Heterogeneous Catalysis: Fundamentals and Applications	4
2	<b>CHP-603</b>	Applied Electrochemistry	4
3	<b>CHC-651</b>	Discipline Specific Dissertation	16



**Name of the Programme:** M.Sc. Part-II (Physical Chemistry)

**Course Code:** CHP-600      **Title of the course:** Practical Course in Physical Chemistry - III

**Number of Credits:** 4

**Effective from AY:** 2023-24

<b>Prerequisites for the course:</b>	Should have studied Physical chemistry practical course at M.Sc. Part-I.	
<b>Course Objectives:</b>	1. To introduce concepts of Kinetics and Thermodynamics 2. To introduce concepts of Surface science and Catalysis 3. To introduce various concepts of Electrochemistry 4. Introduction to the use of computers and computational tools in chemistry	
<b>Contents</b>	<p><i>Note: A minimum of 7 experiments from each Unit I-III are to be completed.</i></p> <p><b>Unit - I. Instrumental</b></p> <p>a. To determine the redox potential of <math>\text{Fe}^{2+}/\text{Fe}^{3+}</math> system using rotating disk voltammetry method.</p> <p>b. To determine the instability constant of the reaction <math>[\text{Ag}(\text{NH}_3)_2] \rightarrow \text{Ag} + 2\text{NH}_3</math> potentiometrically.</p> <p>c. To determine the transport number of ions using moving boundary method.</p> <p>d. To verify Nernst equation and determine the standard oxidation potential of copper and zinc electrodes.</p> <p>e. To study effect of ionic strength on activity coefficient of <math>\text{Ag}^+</math> ions.</p> <p>f. To investigate the reaction kinetics between Potassium Persulphate and Potassium Iodide colorimetrically.</p> <p>g. To determine the equivalent conductance of a strong electrolyte (KCl) at several concentrations and verify Onsager's equation.</p> <p>h. To estimate the concentration of Sulphuric acid, Acetic acid and Copper sulphate in a given solution conductometrically.</p> <p>i. To determine the concentration of <math>\text{Fe}^{2+}</math> ions by titrating with potassium dichromate conductometrically.</p> <p>j. To study the kinetics of hydrolysis of tertiary butyl chloride by conductometry.</p> <p>k. To determine the half wave potential of <math>\text{Cu}^{2+}/\text{Cd}^{2+}/\text{Zn}^{2+}</math> by using polarography.</p> <p>l. To study the effect of sol-gel and hydrothermal method of synthesis on crystallite size and surface area of a semiconductor catalyst.</p> <p>m. To investigate the effect of catalyst loading on photocatalytic degradation of azo dye using semiconductor catalyst.</p> <p>n. To study the stress-strain response of polymeric materials and compare their strength.</p>	No of hours  40

	<p>o. To determine the degradation rate of the polymers using thermogravimetric methods.</p> <p>p. To determine the curie temperature of conducting polymer samples.</p> <p>q. To determine the resistivity of polymeric material using four probe method.</p>	
	<p><b>Unit - II. Non-Instrumental</b></p> <p>a. To determine the critical micelle concentration of three types of surfactants using stalagmometer.</p> <p>b. To determine the partial molal volume of sodium chloride-water, ethanol-water and methanol-water system by apparent molal volume method.</p> <p>c. To study the effect of surfactants on surface tension of water using stalagmometer.</p> <p>d. To study the variation of viscosity with composition of mixtures and to verify the formation of compounds by Oswald's viscometer.</p> <p>e. To study the effect of pH on the kinetics of iodination of Aniline.</p> <p>f. To study the kinetics of reaction between H<sub>2</sub>O<sub>2</sub> and KI (clock reaction).</p> <p>g. To study the kinetics of rapid reaction between Bromine and Iodine in aqueous media.</p> <p>h. To investigate the autocatalytic reaction between Potassium Permanganate and Oxalic acid.</p> <p>i. To study the electroless deposition of Ni on non-conductor substrate and to determine the rate of deposition.</p> <p>j. To study the variation in catalytic activity of three different metal oxides for H<sub>2</sub>O<sub>2</sub> decomposition reaction.</p> <p>k. To investigate the effect of pH on adsorptive separation of azodye from water using MCM-41.</p>	40
	<p><b>Unit - 3. Computational Chemistry</b></p> <p>a. To generate a mark sheet and understand various features of spreadsheets.</p> <p>b. To generate a plot for a given function such as solutions of 1D box, harmonic oscillator, H-like atom wave functions, Gaussians distributions etc.</p> <p>c. To write a computer program to obtain equivalence point in pH metry and potentiometric experiments (derivative method).</p> <p>d. To write a computer program to find percent composition for various atoms of a given molecular formula.</p> <p>e. To write a computer program to obtain slope and intercept for linear data using least square fit method.</p> <p>f. To write a computer program to obtain center of mass of a given molecule and moment of inertia, hence obtain classification of the</p>	40

	<p>given molecule.</p> <p>g. To write a computer program to find out various parameters for data analysis viz. minimum, maximum, average, standard deviation, variance, covariance, correlation coefficient, frequency distribution etc.</p> <p>h. To write a computer program to obtain thermodynamic probability.</p> <p>i. To write a computer program to obtain degeneracy of a given energy level for a particle in a cube.</p> <p>j. Calculate the ground state energy of hydrogen atom using various basis sets using <i>ab-initio</i> program.</p> <p>k. Calculate and interpret the IR, RAMAN and NMR spectra of simple organic molecules using <i>ab-initio</i> program.</p>	
<b>Pedagogy:</b>	Mainly pre-labs / practicals or a combination of some of these could also be used to some extent.	
<b>References / Readings:</b>	<ol style="list-style-type: none"> <li>1. A. Finlay and J.A. Kitchener, Practical Physical Chemistry, Longman Publisher, 1963.</li> <li>2. A. M. James, Practical Physical Chemistry, Longman Publisher, 1974.</li> <li>3. D.P. Shoemaker and C.W. Garland, Experimental Physical Chemistry, McGraw-Hil, 1981.</li> <li>4. J. B. Yadav, Advance Practical Physical Chemistry, Krishna Educational Publishers, 2014.</li> <li>5. S.Attila, and N. S. Ostlund. Modern quantum chemistry: introduction to advanced electronic structure theory. Courier Corporation, 2012.</li> <li>6. P.P. Morajkar, A. P. Naik, S. T. Bugde, B. R. Naik, CH-20: Photocatalytic and microbial degradation of Amaranth dye, Advances in Biological Science Research-A Practical Approach 2019, 327-345, Academic Press.</li> <li>7. J.B. Foresman, E. Frisch, Exploring Chemistry with Electronic Structure Methods: A Guide to Using Gaussian, 2nd Ed. Gaussian, 1996</li> </ol>	
<b>Course Outcomes:</b>	<ol style="list-style-type: none"> <li>1. Student should be able to apply the concepts of physical chemistry in M.Sc. Dissertations.</li> <li>2. Students shall be equipped with practical skills needed for research and development.</li> <li>3. Students will understand the instrumental and non-instrumental methods of analysis.</li> <li>4. Students will understand use of computers and computational tools in chemistry.</li> </ol>	

**Name of the Programme:** M.Sc. Part-II (Physical Chemistry)

**Course Code:** CHP-601      **Title of the course:** Practical Course in Physical Chemistry - IV

**Number of Credits:** 4

**Effective from AY:** 2023-24

<b>Prerequisites for the course:</b>	Should have studied Physical chemistry practical course at M.Sc. Part-I.	
<b>Course Objectives:</b>	1. To introduce concepts of Kinetics and Thermodynamics 2. To introduce concepts of Surface science and Catalysis 3. To introduce various concepts of Electrochemistry 4. Introduction to the use of computers and computational tools in chemistry	
<b>Content</b>	<b>Unit - I. Instrumental</b> a. To estimate the concentration of glucose calorimetrically. b. To determine the redox potential of $\text{Fe}^{3+}/\text{Fe}^{2+}$ system using rotating disk voltammetry method. c. To determine the transport number of ions using moving boundary method. d. To verify Nernst equation and determine the standard reduction potential of Ag and Zn electrodes. e. To determine the equivalent conductance of a strong electrolyte (NaCl) at several concentrations and verify Onsager's equation. f. To estimate the concentration of Hydrochloric acid, Monochloro acetic acid and Copper sulphate in a given solution conductometrically. g. To determine the half wave potential of $\text{Ni}^{2+}/\text{Cd}^{2+}/\text{Cu}^{2+}$ by using polarography. h. To study the effect of precipitation and hydrothermal method of synthesis on acidic sites of a semiconductor catalyst using $\text{NH}_3$ TPD method. i. To investigate the effect of solution pH on photocatalytic degradation of methylene blue using semiconductor photocatalyst. j. To determine the curie temperature of polyaniline.	No of hours 40
	<b>Unit II. Non-Instrumental</b> a. To determine the critical micelle concentration of Sodium dodecyl sulphate, Cetrimonium bromide using stalagmometer. b. To study the kinetics of the reaction between acetone and Iodine using titrimetry. c. To study the effect of pH on the kinetics of iodination of aniline. d. To study the kinetics of Briggs Rauscher reaction (oscillatory	40

<p>reaction).</p> <ol style="list-style-type: none"> <li>e. To study the kinetics of rapid reaction between Bromine and Iodine in aqueous media</li> <li>f. To investigate the autocatalytic reaction between Potassium Permanganate and Citric acid.</li> <li>g. To study the electroless deposition of Cu on alpha-alumina and to determine the rate of deposition.</li> <li>h. To compare the catalytic activity of MnO<sub>2</sub>, NiO with Degussa-P25 towards H<sub>2</sub>O<sub>2</sub> decomposition reaction.</li> <li>i. To investigate the effect of pH on adsorptive separation of Amaranth dye from water over NiO catalyst.</li> <li>j. To determine the radius of a glycerol molecule by viscosity measurements.</li> </ol>	
<p><b>Unit III. Computational Chemistry</b></p> <ol style="list-style-type: none"> <li>a. To write a computer program to find out various parameters for data analysis viz. minimum, maximum, average, standard deviation, variance, covariance, correlation coefficient, frequency distribution etc.</li> <li>b. To write a computer program to obtain slope and intercept for linear data using least square fit method</li> <li>c. To analyze the Gaussian output files and extracts molecular coordinates.</li> <li>d. To construct and optimize the molecular structure of H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub> and HOF using Gaussian/ NWCHEM and calculate bond distances and bond angles.</li> <li>e. To obtain the transition state of the reaction between CH<sub>3</sub>Br and OH<sup>-</sup> ions using Gaussian/ NWCHEM.</li> <li>f. To study the effect of solvent on the transition state of the reaction between CH<sub>3</sub>Br and OH<sup>-</sup> using Gaussian/ NWCHEM.</li> <li>g. To study the thermochemistry of the reaction between CH<sub>3</sub>Cl and OH<sup>-</sup> using Gaussian/ NWCHEM.</li> <li>h. To generate a plot for a given function such as solutions of 1D box, harmonic oscillator, H-like atom wave functions, Gaussians distributions etc.</li> <li>i. To write a computer program to obtain degeneracy of a given energy level for a particle in a rectangular box.</li> <li>j. Calculate the ground state energy of hydrogen atom using various basis sets using Gaussian 16 program.</li> </ol> <p><i>Note: A minimum of 7 experiments from each Unit I-III are to be completed.</i></p>	40

<b>Pedagogy:</b>	Mainly pre-labs / practicals or a combination of some of these could also be used to some extent.
<b>References / Readings:</b>	<ol style="list-style-type: none"> <li>1. A. Finlay and J.A. Kitchener, Practical Physical Chemistry, Longman Publisher, 1963.</li> <li>2. A. M. James, Practical Physical Chemistry, Longman Publisher, 1974.</li> <li>3. D.P. Shoemaker and C.W. Garland, Experimental Physical Chemistry, McGraw-Hil, 1981.</li> <li>4. J. B. Yadav, Advance Practical Physical Chemistry, Krishna Educational Publishers, 2014.</li> <li>5. S. Attila, and N.S. Ostlund. Modern quantum chemistry: introduction to advanced electronic structure theory. Courier Corporation, 2012.</li> <li>6. P. P. Morajkar, A. P. Naik, S. T. Bugde, B. R. Naik, CH-20: Photocatalytic and microbial degradation of Amaranth dye, Advances in Biological Science Research-A Practical Approach 2019, 327-345, Academic Press.</li> <li>7. J.B. Foresman, E. Frisch, Exploring Chemistry With Electronic Structure Methods: A Guide to Using Gaussian, 2nd ed. Gaussian, 1996.</li> </ol>
<b>Course Outcomes:</b>	<ol style="list-style-type: none"> <li>1. Student should be able to apply the concepts of physical chemistry in M.Sc. Dissertations.</li> <li>2. Students shall be equipped with practical skills needed for research and development.</li> <li>3. Students will understand the instrumental and non-instrumental methods of analysis.</li> <li>4. Students will understand use of computers and computational tools in chemistry.</li> </ol>

**Name of the Programme:** M.Sc. Part-II (Physical Chemistry)

**Course Code:** CHP-602      **Title of the course:** Heterogeneous Catalysis: Fundamentals and Applications

**Number of Credits:** 4

**Effective from AY:** 2023-24

<b>Prerequisites for the course:</b>	Students should have studied Chemistry courses at MSc Part-I.	
<b>Course Objectives:</b>	1. To introduce concepts of surface science and catalysis. 2. To provide fundamental knowledge of theories that govern heterogeneous catalytic reactions. 3. To introduce newer methods of synthesizing nanocatalysts and its characterization. 4. To introduce latest developments about application of catalyst in environment and energy sector.	
<b>Concepts</b>	1. <b>Basic Concepts</b> a. General Introduction: Catalysis and activation energy. Heterogeneous reactions with suitable illustrations. Catalytic activity, selectivity and stability. Steps in a heterogeneous catalytic reaction. Factors affecting rate of reaction such as temperature, flow rates, molar composition etc. b. Adsorption and Surface Area: Cause of adsorption. No of molecules striking the surface and sticking probability. Types of adsorption and potential energy profiles for adsorption of H <sub>2</sub> . Adsorption isotherms for gases and solutes. Basic types of BET isotherms. Gibbs adsorption equation and changes in surface tension. Free energy, enthalpy and entropy of adsorption. Chemisorption of H <sub>2</sub> , O <sub>2</sub> and CO. Surface area and Porosity: Determination of surface area. Porosity and pore size distribution. c. Classification of catalysts based on electrical conduction. Adsorption on specific crystal planes; geometric factor in catalysis: Balandin's multiplet theory and Valence angle conservation. Cumulative & depletive adsorption, Electronic effect in catalysis by metals. Role of diffusion in catalysis.	No of hours 20
	2. <b>Kinetics and mechanisms of catalyzed reactions</b> Kinetics of catalyzed reactions and rate expressions. Mechanism of catalyzed reactions obeying Langmuir-Hinshelwood, Eley-Rideal and Mars van Krevelen models with suitable examples.	5

	<p><b>3. Preparation of Catalysts</b>  Various methods for preparation of bulk catalysts: Precipitation method, Impregnation method catalyst impregnation with or without interaction between support and catalyst. Synthesis of microporous solids. Synthesis of mesoporous solids.</p>	5
	<p><b>4. Thermal and Spectroscopic Methods in Heterogeneous Catalysis</b>  Characterization of the catalysts by temperature programmed desorption using probes such as ammonia and pyridine molecules. Characterization of surface area using BET method. Characterization of adsorbed molecules/intermediates by IR spectroscopy and XPS. Introduction to EXAFS and Mössbauer spectroscopy in characterizing catalysts.</p>	10
	<p><b>5. Zeolite based Catalysis and industrial applications</b>  Structure building in zeolites such ZSM-5. Nature of active sites and their characterization. Role of Zeolite acidity and Shape Selectivity in catalytic reactions. Zeolite based catalysis in MTG process.</p>	5
	<p><b>6. Semiconductor catalysis and its application in energy and environmental sector</b>  Introduction to semi-conductor surface and catalysis with application in photocatalytic water splitting and CO<sub>2</sub> reduction to value added chemicals. Case studies on photocatalytic degradation of dyes. Practical demonstration of photocatalytic treatment of laboratory waste water contaminated with dyes, adsorptive separation and kinetic analysis.</p>	10
	<p><b>7. Electrocatalysis and applications</b>  Basic electro-catalytic concepts, comparison of electro-catalysts. Electrocatalytic water splitting reaction. Role of catalytic materials in energy storage applications.</p>	5
<b>Pedagogy:</b>	Mainly lectures, tutorials, assignments, demonstration, self-study or a combination of some of these could also be used to some extent.	
<b>Reference / Readings:</b>	<ol style="list-style-type: none"> <li>1. D. K. Chakrabarty and B. Viswanathan, Heterogeneous Catalysis, New Age International Publishers, 2008.</li> <li>2. G. A. Somorjai, Introduction to Surface Chemistry and Catalysis, John Wiley, 2002.</li> <li>3. M. Thomas and W. J. Thomas, Principles and Practice of Heterogeneous Catalysis, VCH Publishers, 1996.</li> <li>4. P.P. Morajkar, A. P. Naik, S. T. Bugde, B. R. Naik, CH-20:</li> </ol>	



	<p>Photocatalytic and microbial degradation of Amaranth dye, <i>Advances in Biological Science Research-A Practical Approach</i> 2019, 327-345, Academic Press.</p> <p>5. B.H.R. Suryanto, Y. Wang, R. K. Hocking, Overall electrochemical splitting of water at the heterogeneous interface of nickel and iron oxide. <i>Nature Commun.</i> 2019, 10, 5599.</p> <p>6. A. V. Salkar; S. V. Bhosale; P. P. Morajkar, CH-6: Nanostructured <math>WO_{3-x}</math> Based Advanced Supercapacitors for Sustainable Energy Applications, <i>Advances in Metal Oxides and Their Composites for Emerging Applications</i>; Elsevier, 2022, 213–238. ELSEVIER.</p> <p>7. A.V. Salker, <i>Catalysis: Principles and Basic Concepts</i>, Scientific International, 2019.</p>
<p><b>Course Outcomes:</b></p>	<ol style="list-style-type: none"> <li>1. Students will be able to design a nanocatalysts for adsorption application.</li> <li>2. Students will be able to interpret characterization data of nano catalysts.</li> <li>3. Students will be able to design a catalyst for environmental and energy applications.</li> <li>4. Students will learn about semiconductor catalysis.</li> </ol>

**Name of the Programme:** M.Sc. Part-II (Physical Chemistry)

**Course Code:** CHP-603      **Title of the course:** Applied Electrochemistry

**Number of Credits:** 4

**Effective from AY:** 2023-24

<b>Prerequisites for the course:</b>	Students should have studied Chemistry courses at M.Sc. Part-I.	
<b>Course Objective:</b>	1. Introduction to core concepts of electrochemical applications 2. To enable design and development of electrochemical systems for specific applications 3. Introduction of applications and working principles of electrochemical devices in day-to-day life eg. batteries, solar cells, capacitors	
<b>Content</b>	<b>1. Electroanalytical Techniques</b> Principles and applications of the following techniques: a. Amperometry b. Cyclic voltammetry c. Voltammetry at rotating disk electrodes d. Electrochemical impedance spectroscopy	No of hours  10
	<b>2. Corrosion</b> a. Corrosion and electrochemical kinetics. Pourbaix diagrams Mechanism of electrochemical corrosion. b. Mixed electrode and mixed potential. Overpotential and polarization. c. Current density – potential curves and determination of corrosion current density. d. Hydrogen and oxygen overpotentials and corrosion e. Types of electrolytic corrosion and forms of localized corrosion, practical cases of corrosion. Corrosivity and passivity f. Corrosion prevention. Corrosion inhibitors. Corrosion Testing. Cathodic and anodic protection g. Polarization tests and impedance spectroscopic measurements.	10
	<b>3. Electrochemical Power Sources: Batteries, Fuel Cells and Supercapacitors</b> a. Electrical characteristics of batteries. Batteries with aqueous and non-aqueous electrolytes. Types of batteries, Ohmic losses and thermal processes in batteries. Next generation batteries: Lithium ion batteries, Sodium ion batteries b. Thermodynamic aspects of fuel cells. Working principles of fuel cells. Types of fuel cells: polymer electrolyte membrane fuel cells (PEMFCs), direct liquid fuel cells (DLFCs), molten carbonate fuel cells (MCFCs), solid oxide fuel cells (SOFCs), alkaline fuel cells (AFCs) c. Properties of electrical double layer capacitors. Energy density.	10

	Power density. Electrochemical supercapacitors with carbon electrodes. Pseudocapacitor electrodes and supercapacitors. Hybrid supercapacitors: metal oxide (MeO <sub>x</sub> /C) and electronically conducting polymer/carbon (ECP/C) types	
	<p><b>4. Electrocatalysis and Electrochemical Sensors</b></p> <p>a. Introductory aspects to fuel cell electrocatalysis. Electrochemical energy conversion.</p> <p>b. Electrocatalytic surfaces. Structure stability and mass transport on electrode surfaces, Basic electrocatalytic mechanisms and kinetics</p> <p>c. Electrochemistry of methanol electrooxidation</p> <p>d. Types of electrocatalysts, Electrochemistry of ORR and HER</p> <p>e. Introduction to principles of chemical sensing; Signal transduction; Physico-chemical and biological transducers; Sensor types and technologies, Chemically modified electrodes for sensing</p> <p>f. Types of electrochemical sensors (voltammetric, potentiometric, amperometric, impedimetric), Methods for sensors fabrication: self-assembled monolayers, screen printing, photolithography, microcontact printing, MEMS</p> <p>g. Test-strips for glucose monitoring</p>	15
	<p><b>5. Photoelectrochemical devices</b></p> <p>a. Photoelectrochemical cell design, photoconversion efficiency, photoelectrochemical water splitting</p> <p>b. Principles and applications of dual-working-electrode photoelectrochemistry</p> <p>c. Principles and working of first and second generation solar cells</p> <p>d. Fabrication and operational principles of third generation photovoltaics: perovskite solar cells, dye-sensitized solar cells, quantum dot solar cells</p> <p>e. Tandem photovoltaic cells</p>	15
<b>Pedagogy</b>	Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
<b>References / Readings</b>	<p>J.O.M. Bockris and A.K.N. Reddy, <del>Modern Electrochemistry, Vol 1, 2 and 3, Kluwer Academic Publishers, New York, 2002</del></p> <p>A. Vincent &amp; B. Sacrosati, <del>Modern Batteries, John Wiley, New York, 1997.</del></p> <p>J.O.M. Bockris &amp; S. Srinivasan, <del>Fuel cells: Their Electrochemistry, McGraw-Hill Book Co., 1969.</del></p> <p>E. Santos &amp; W. Schmickler, <del>Catalysis in Electrochemistry: From Fundamental to Strategies for Fuel Cell Development, Wiley, 2011</del></p>	

	<p>J. Lipkowski &amp; P. N. Ross, <i>Electroanalysis</i>, Wiley-VCH, New York, 1998</p> <p>A.J. Bard, M. Stratmann, S. Licht, <i>Fundamentals of Electrochemistry, Semiconductor Electrodes and Photoelectrochemistry</i>, Wiley-VCH, 2002.</p> <p>S. Gimenez &amp; J. Bisquert, <i>Photoelectrochemical Solar Fuel Production: From Basic Principles to Advanced Devices</i>, Springer International Publishing, 2016</p> <p>V. S. Bagotsky, A. M. Skundin &amp; V. M. Valtschik, <i>Electrochemical Power Sources: Batteries, Fuel Cells, and Supercapacitors</i>, John Wiley &amp; Sons, Inc., New Jersey, 2015</p> <p>N. Perez, <i>Electrochemistry and Corrosion Science</i>, Kluwer Academic Publishers, Boston, 2004.</p> <p>C. Jiang, S. J. A. Moniz, A. Wang, B. Peng, I. Lang, Photoelectrochemical devices for solar water splitting – materials and challenges, <i>Chem. Soc. Rev.</i>, 2017, 46, 4645-4660.</p> <p>M. Stanley, W. R. F. Savinell, T. Zawodzinski, <i>Introduction: Batteries and Fuel Cells</i>, <i>Chem. Rev.</i>, 2004, 104, 10, 4243</p> <p>E. Bakker, Y. Qin, <i>Electrochemical Sensors</i>, Eric Bakker, <i>Anal. Chem.</i> 2006, 78, 3965-3984</p>
<p><b>Course Outcome:</b></p>	<ol style="list-style-type: none"> <li>1. Students will be in a position to apply these concepts during the lab course in physical chemistry.</li> <li>2. Students will gain knowledge and apply the same in electrochemistry dissertation and research work.</li> <li>3. Students will learn about electrochemical sensors.</li> <li>4. Students will learn about fuel cells.</li> </ol>

**Name of the Programme:** M.Sc. Part-II (Physical Chemistry)

**Course Code:** CHP-621      **Title of the course:** Solid State Chemistry: Concepts and Applications

**Number of Credits:** 4

**Effective from AY:** 2023-24

<b>Prerequisites for the course:</b>	Students should have studied the chemistry/physics courses at M.Sc. Part-I	
<b>Course Objective:</b>	1.To introduce concepts and provide fundamental knowledge of principles of materials chemistry, characterization methods and techniques 2. To provide fundamental knowledge of molecular solids, description of crystal chemistry and classification of phase structure and significance of imperfections in solids. 3. To provide basic understanding of temperature dependence of crystal structure, phase modifications and its influence on magnetic and electronic properties of materials 4. To provide a comparative evaluation of data obtained from various techniques and their use in elucidating the chemical and morphological structure of solid materials	
<b>Content</b>	<b>1. Solid State: Introduction</b> General Principles and experimental procedure. Various methods in solid-state synthesis c. Kinetics of solid-state reactions, ion exchange, and intercalation reactions.	No of hours 6
	<b>2. Crystal Chemistry and X-Ray Diffraction:</b> a. Crystal systems, Bravais lattices and Quasicrystals. b. Ionic structures and covalent networks. c. Some important structure types –rock salt, zinc blende, wurtzite, nickel arsenide, rutile, and van der Waals heterostructures. d. Factors that Influence Crystal Structures: valences and coordination numbers. e. Significance of radius ratio rule and non-bonding electron effects. f. Powder X-ray diffraction experiment, instrumentation g. Introduction to single-crystal X-ray diffraction. Applications of high-temperature powder diffraction. h. Identification of crystal phases and evaluation of lattice characteristics	15
	<b>3. Crystal Defects and non-stoichiometry</b> a. Types of defects. Point defects and thermodynamics.	6

	<p>b. Colour Centres, vacancies, and interstitials in non-stoichiometric crystals.</p> <p>c. Dislocations, mechanical properties, and reactivity of solids</p>	
	<p><b>4. Phase Diagrams and Phase Transitions</b></p> <p>a. Basic Concepts and definitions.</p> <p>b. Three-component condensed systems. Martensitic transformations. Order-disorder transitions.</p>	6
	<p><b>5. Electronic Properties and Band Theory</b></p> <p>a. Electronic structure and band theory of solids. Band structure of metals and semiconductors.</p> <p>b. Magnetic properties of transition metal oxides and applications Electrical conductivity, free electron theory, fermi energy, insulators, semiconductor and conductors, band theory of semiconductor, Brillouin zones, Hall effect, the Seebeck effect, Superconductivity, BCS theory, Meissner effect, high temperature superconductor.</p>	6
	<p><b>6. Electronic Microscopic Techniques</b></p> <p>a. Introduction to Electron Microscopy: Generation of electron beam, elastic and inelastic scattering of electrons by atoms.</p> <p>b. Scanning Electron Microscopy (SEM): Instrumentation, optics, resolution and compositional imaging, Preparation of specimen, crystallographic information from SEM and Environmental Scanning Electron Microscopy (E-SEM)</p> <p>c. High Resolution Transmission Electron Microscopy (HR-TEM): Instrumentation, contrast mechanism, high voltage and Scanning Transmission Electron microscopy (STEM), preparation of specimen and data interpretation.</p> <p>d. Cryogenic Electron Microscopy (Cryo-TEM)</p>	8
	<p><b>7. X-Ray Spectroscopy</b></p> <p>a. Intensities: scattering of X-Rays and factors that affect intensities, powder x-ray pattern</p> <p>b. XRF, X-ray absorption near edge structure (XANES) and extended x-ray absorption fine structure (EXAFS): Absorption coefficient, absorption edges, resonance emission, extended absorption and photoelectron scattering.</p> <p>c. X-ray photoelectron spectroscopy (XPS): Surface analysis, sensitivity and specificity, photoelectron intensities, binding energies and spectra analysis</p> <p>c. Instrumentation and design, characterization of transition metal oxides.</p>	8
	<p><b>8. Thermal Analysis</b></p> <p>a. Thermogravimetric analysis, Differential Thermal Analysis</p> <p>b. Differential scanning calorimetry</p>	5

	c. Application to the characterization of materials
<b>Pedagogy</b>	Mainly lectures and tutorials. Seminars / term papers / assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.
<b>References / Readings</b>	<p>A. R. West, Solid State Chemistry and Its Applications, John Wiley &amp; Sons 2003.</p> <p>H. V. Keer, Principles of the Solid State, New Age International Publishers, 1993.</p> <p>C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, McGraw-Hill Education (India) Private Limited, 1994</p> <p>P. van der Heide, X-ray Photoelectron Spectroscopy: An Introduction to Principles and Practices, John Wiley &amp; Sons, Inc. 2012</p>
<b>Course Outcome:</b>	<ol style="list-style-type: none"> <li>1. Students will be in a position to explain the concept of solid state synthesis, identify different crystal structure</li> <li>2. Students will be in a position to explain the design of the instrumental techniques, data acquisition, and analysis to elucidate structural information of solid materials</li> <li>3. Students will be able to apply the concepts learned to make the best choice of a characterization technique(s) for elucidation of unknown solids under investigation.</li> <li>4. Students will learn about electronic microscopic techniques.</li> </ol>

**Name of the Programme:** M.Sc. Part-II (Physical Chemistry)

**Course Code:** CHP-622      **Title of the course:** Nanoscience: Concepts and Applications

**Number of Credits:** 4

**Effective from AY:** 2023-24

<b>Prerequisites for the course:</b>	Students should have studied the M.Sc. I courses of chemistry/ physics/ biological sciences	
<b>Course Objective:</b>	1. Introduction of various concepts for nanoscience. 2. Introduction of various synthesis methods of nanomaterials. 3. Introduction of various characterisation techniques and application study of nanomaterials	
<b>Content</b>	<b>1. Essential Concepts and definitions</b> Nanoscale, quantum effects, thermal properties of nanomaterials, optical properties of nanomaterials, electrical properties of nanomaterials, Metallic nanowires and quantum conductance, Surface to volume ratio of nanoparticles, surface effects and surface energy on Nanoparticle surface. Chemistry of solid surfaces.	No of hours 15
	<b>2. Methods of nanomaterial synthesis</b> Principles, methods, formation mechanism and structures of nanomaterials for: Gas-phase processes, Liquid-phase processes, Solid-phase processes, Self-assembly processes	10
	<b>3. Characterization techniques</b> Beam Probe methods (SEM, TEM), Scanning probe method (STM, AFM), optical method: principle, sample preparation technique and applications. Case studies: core-shell nanoparticles, metal nanoparticles, composite nanoparticles.	10
	<b>4. Important nanomaterials</b> <b>Silica:</b> discussion of sol-gel and liquid crystal synthesis method, self-assembly of colloidal silica particles, photoluminescence property of opals, different surface functionalization methods and application study. <b>Gold:</b> Different colloidal synthesis methods, self-assembly methods, surface Plasmon resonance (SPR) of colloidal gold nanoparticles surface functionalization strategies and application study. <b>CdSe:</b> Different synthesis methods, synthesis of core-shell particles, Study of CdSe excitons and CdSe quantum dots, functionalization and application study.	15



	<p><b>Iron oxide (Fe<sub>3</sub>O<sub>4</sub>):</b> Different synthesis methods, Superparamagnetism property of nanoparticles, Hysteresis and magnetisation of Fe<sub>3</sub>O<sub>4</sub> nanomaterial, catalytic and Biomedical applications.</p> <p><b>Carbon:</b> synthesis methods for carbon nanotubes, Graphene and Buckminster fullerene, structural study of these materials, electrical property study of these materials, surface functionalization strategies and application study.</p>	
	<p><b>5. Applications of nanomaterials</b> Heterogeneous catalysts for the synthesis of fine chemicals, Polymer vesicles for drug delivery, Surface-modified metal nanoparticles for recognition of toxic organic molecules, Use of nano TiO<sub>2</sub> and ZnO for water and air pollution control, Carbon Materials for Energy Storage, Thermoelectric Nanomaterials</p>	8
	<p><b>6. Nanomaterials: risk, toxicity</b> Toxicity of inorganic-based, carbon-based, composite-based nanomaterials, environmental, health, and safety issues.</p>	2
<b>Pedagogy</b>	Mainly lectures and tutorials. Seminars / term papers / assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
<b>References / Readings</b>	<p>L. Cademartiri and G.A.Ozin, <i>Concepts of Nanochemistry</i>, Wiley-VCH, 2009.</p> <p>C.N.R. Rao and A. Govindaraj, <i>Nanotubes and nanowires</i>, Royal society of Chemistry, 2005.</p> <p>G. Cao, <i>Nanostructures and Nanomaterials</i>, Imperial College Press, 2004.</p> <p>J. M. Tour, <i>Molecular Electronics</i>, Imperial College Press, 2004</p> <p>H. S. Nalwa (Ed), <i>Encyclopedia of Nanoscience and Nanotechnology</i>, American Scientific Publishers, 2004.</p> <p>E. Roduner, <i>Nanoscope Material: Size, Shape and Properties</i>, RSC Publishing, Cambridge, 2006.</p> <p>G.A. Ozin and A.C. Arsenault, <i>Nanochemistry: A Chemical Approach to Nanomaterials</i>, RSC Publishing, Cambridge, 2005.</p> <p>C.P. Poole and F.J. Owens, <i>Introduction to Nanotechnology</i>, John Wiley and Sons, 2003.</p> <p>B. Zhang, <i>Physical Fundamentals of Nanomaterials</i>, Chemical industry press, 2018.</p> <p>C. M. Hussain, <i>Handbook of Nanomaterials and Nanotechnology</i>, Elsevier, 2020.</p> <p>A. Barhoum and A. S. H. Makhlof, <i>Emerging Applications of Nanoparticles and Architecture Nanostructures: Current Prospects and Future Trends</i>, Elsevier, 2018.</p> <p>R.G. Chaudhuri and S. Paria, <i>Core/shell nanoparticles: classes,</i></p>	

	properties, synthesis mechanisms, characterization, and applications, Chemical reviews ACS, 2012, 112, 2373-2433.
<b>Course Outcome:</b>	<ol style="list-style-type: none"><li>1. Students will learn different techniques of synthesis and characterisation of nanomaterials.</li><li>2. Students should be in a position to understand and explain magnetic, electrical, optical and catalytic properties of materials at nanoscale.</li><li>3. Students should be in a position to apply the knowledge of subject for their dissertation and research work.</li><li>4. Students will learn about applications of nanomaterials.</li></ol>

**Name of the Programme:** M.Sc. Part-II (Physical Chemistry)

**Course Code:** CHP-623      **Title of the course:** Physical aspects of Polymer Chemistry

**Number of Credits:** 4

**Effective from AY:** 2023-24

<b>Prerequisites for the course:</b>	Students should have studied chemistry courses at M.Sc. I.	
<b>Course Objective:</b>	1. To introduce physical and chemical aspects of polymer chemistry. 2. To introduce kinetics of polymerization, different characteristics of polymers, applications of biodegradable and thermoset polymers.	
<b>Content</b>	<b>1. Introduction to polymer chemistry</b> a. Historical development in polymer chemistry, polymer industry in 21 <sup>st</sup> century. b. Classification of polymers, Polymer nomenclature. Polymer tacticity, geometry and stereoregularity. c. Thermoplastics and thermosets- Plastics, elastomers, fibres. Concepts of Functionality, terminal groups, homopolymers and copolymers etc. d. Addition and condensation polymers- - linear, branched, IPN and cross-linked polymers-graft and block co-polymers.	No of hours  10
	<b>2. Molecular weight and other classification of polymers</b> a. Polymer molecular weight, arithmetic mean – Number average, weight average, polydispersity and Polydispersity index (PDI) b. Degree of polymerization and its impact on MW and mechanical properties. c. Amorphous and crystalline polymers. Methods of analysis of crystallinity. d. Glass transition temperature and other thermal transitions. Importance of $T_g$ –Plasticizers and their action. Secondary bonding forces in polymers.	10
	<b>3. Polymerization techniques</b> a. Methods of polymerization (homogeneous and heterogenous polymerization) b. Co-ordination polymerization, Zeigler–Natta and other catalytic polymerization techniques. c. Atom transfer radical polymerization (ATRP), Reversible addition-fragmentation chain transfer polymerization (RAFT). d. Advantages and disadvantages of polymerization techniques	10

	<p><b>4. Polymer molecular weight and its determination</b></p> <p>a. Molecular weight averages: Arithmetic mean; Number average molecular weight; Weight average molecular weight.</p> <p>b. Molecular weight determination: end group analysis; colligative property measurement; dilute solution viscosity; Mark-Houwink-Sakurada (MHS) equation.</p> <p>c. Gel permeation Chromatography</p>	8
	<p><b>5. Kinetics of polymerization</b></p> <p>Introduction; Free radical chain polymerization; Equation for kinetic chain length; degree of polymerization; ceiling temperature, Anionic polymerization, Cationic polymerization, Polycondensation; Non catalyzed polycondensation; catalyzed polycondensation</p>	8
	<p><b>6. Characterization of polymers by various techniques</b></p> <p>a. Instruments and testing methods for polymer characterization</p> <p>b. Characterization of chemical structure of polymers: by chemical reaction methods; IR spectroscopy; Raman spectroscopy; UV-Visible spectroscopy; NMR and ESR spectroscopy.</p> <p>c. Characterization of polymer morphology and Physical structure of Polymers: TEM; X-ray scattering; WAXS; SAXS; AFM.</p> <p>d. Characterization of Thermal Properties of Polymers: Differential thermal analysis (DTA), Physical transitions, melting thermograms, Melt crystallization; Differential Scanning coulometry (DSC); Thermogravimetric analysis (TGA).</p>	14
<b>Pedagogy</b>	Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
<b>References / Readings</b>	<p>V. R. Gowariker, N. V. Viswanathan, and I. Sreedhar, <i>Polymer Science</i>, Wiley Eastern Ltd., 1986.</p> <p>P. Bahadur and N. V. Sastry, <i>Principles of Polymer science</i>, Narosa Publishing House, 2003.</p> <p>J. R. Fried, <i>Polymer Science and Technology</i>, PHI Pvt Ltd, 2000</p> <p>R. Sinha, <i>Outlines of Polymer Technology- Manufacture of Polymers</i>, PHI Pvt Ltd., 2000.</p> <p>R. Sinha, <i>Outlines of Polymer Technology- Processing Polymers</i>, PHI Pvt Ltd., 2003.</p>	

	<p>J. A. Brydson, <i>Plastic Materials</i>, New York, 1979, 3<sup>rd</sup> edition.</p> <p>J. Urbanski, W. Czerwinski, K. Janicka, F. Majewska, and H. Zowall, <i>Handbook of analysis of synthetic polymers and plastics</i>, John Wiley, 1977.</p> <p>K. Y. Saunders, <i>Organic polymer chemistry</i>, Chapman and Hall, UK, 1976.</p> <p>R. W. Lenz, <i>Organic chemistry of synthetic high polymers</i>, 1967.</p> <p>R. P. Brown, <i>Handbook of plastic technology</i>, George Godwin Ltd., 1981, 2<sup>nd</sup> edition.</p> <p>M. P. Stevens, <i>Polymer Chemistry- An Introduction</i>, Oxford Univ Press, 1990, 2<sup>nd</sup> edition.</p> <p>W. Y. Mijs, <i>New methods in polymer synthesis</i>, Plenum Press Ltd, NY, 1992.</p> <p>P. C. Hiemenz, <i>Polymer chemistry- the basic concepts</i>, Marcell Dekker Inc., 1984.</p> <p>W. R. Moore, <i>Introduction to polymer chemistry</i>, Univ of London Press, 1961.</p> <p>N. P. Cheremisinoff (Ed), <i>Handbook of polymer science and technology</i>, Marcel Dekker Inc., 1989.</p> <p>M. Chanda, <i>Introduction to polymer chemistry, A problem-solving approach</i>, CRC press, 2006.</p> <p>W. F. Su, <i>Principles of Polymer design and synthesis, Volume 82</i>, Springer, 2013.</p> <p>R. M. Silverstein, F. X. Webster, B. I. Kunlay, D. I. Ryan, &amp; D. Samant, V. S. Nadkarni, <i>Spectrometric Identification of Organic Compounds, An Indian Adaptation</i>, 8<sup>th</sup> Ed. Wiley, 2022.</p>
<p><b>Course Outcome:</b></p>	<ol style="list-style-type: none"> <li>1. Students will be able to explain various fundamental concepts of polymer chemistry.</li> <li>2. Students should be in a position to apply the knowledge of polymer chemistry for their dissertation and research work.</li> <li>3. Students should be in a position to apply these concepts during the lab course.</li> <li>4. Students will learn about characterisation of polymers.</li> </ol>

**Name of the Programme:** M.Sc. Part-II (Physical Chemistry)

**Course Code:** CHP-624      **Title of the course:** Colloids and Surface Chemistry

**Number of Credits:** 4

**Effective from AY:** 2023-24

<b>Prerequisites for the course:</b>	Students should have studied chemistry courses at M.Sc. I.	
<b>Course Objective:</b>	1. To introduce some core concepts of colloidal chemistry including DLVO theory, electrokinetic phenomena and diversity in colloids. 2. To introduce fundamental concepts and applications of colloids in day-to-day life.	
<b>Content</b>	<b>1. Colloids and Liquid Surfaces</b> a. Colloids: General introduction, classification and structural characteristics of colloidal system, preparation and purification b. Microscopic picture of liquid surface c. Surface tension and its measurement. Surfactant and reduction of surface tension. Curved liquid surfaces. d. Nucleation theory. e. Surface modification: self-assembly monolayer formation. Physisorption of polymers. Polymerization on surfaces.	No of hours 10
	<b>2. Electrostatic Forces and Electrokinetic Phenomenon</b> a. Electrical double layer. Surface interactions between surfaces (dipole, induced dipole, H-bonding) b. Surface forces: Van der Waals forces between molecules. Surface energy and Hamaker constant. Measurement of surface forces. The DLVO theory c. Charged surfaces such as mercury, silver iodide and oxides. Measurement of surface charge densities d. Electrocapillarity - theory and measurement e. Electrokinetic phenomena: concept of zeta potential. Electroosmosis and streaming potential. Electrophoresis and sedimentation potential. f. Contact angle and its measurements. Wetting and dewetting. Important wetting geometries.	12
	<b>3. Colloidal Stability</b> a. Charged colloids. Electrical charge distribution at interfaces b. Factors affecting colloidal stability. Effect of electrolyte.	8

	<p>c. Flocculation and coagulation. Kinetics of coagulation d. Steric stabilization of solid and liquid colloids</p>	
	<p><b>4. Preparation of colloids</b></p> <p>a. Chemical methods for synthesis of colloids: Sol-gel method, polyol synthesis, plasma enhanced chemical vapor deposition, hydrothermal synthesis</p> <p>b. Colloidal synthesis of semiconductor nanoparticles: Hot-injection synthesis. Synthesis of colloidal core-shell heterostructures</p> <p>c. Surface directed colloidal patterning: Colloidal self-assembly approaches</p> <p>d. Reducing agents in colloidal nanoparticle synthesis</p>	12
	<p><b>5. Surfactants, Micelles, Emulsions and Thin Liquid Films</b></p> <p>a. Classification of surfactants. Solubilization and micelle formation</p> <p>b. Spherical micelles: cmc and influence of temperature. Thermodynamics of micellization. Structure of surfactant aggregates.</p> <p>c. Emulsions: Macro and microemulsions, properties, formation and factors affecting the stability. Evolution and aging. Coalescence and demulsification. Size of droplets. Elasticity of surfactant films.</p> <p>d. Thin films on surfaces of liquids: Introduction and phases. Bubbles and foams. Optical and X-Ray methods to study monolayers.</p> <p>e. Langmuir Blodgett Transfer</p>	13
	<p><b>6. Applications of Colloids in Science, Technology and Industry</b></p> <p>a. Colloids as drug delivery agents</p> <p>b. Colloidal nanocrystals for optical applications and solar cells.</p> <p>c. Biomedical applications</p>	5
<b>Pedagogy</b>	<p>Mainly lectures and tutorials. Seminars / term papers / assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.</p>	
<b>References / Readings</b>	<p>H. J. Butt, K. Graf and M. Kappl, <del>Physics and Chemistry of Interfaces</del>, Wiley-VCH, 2003.</p> <p>A. W. Adamson and A.P.Gast, <del>Physical Chemistry of Surfaces</del>, Wiley-VCH, 1997, 6<sup>th</sup> edition</p> <p>R. D. Vold and M. J. Vold, <del>Colloid and Interface Chemistry</del>, Addison-Wesley, 1983.</p>	

	<p><del>K. S. Birdi, Surface and Colloid Chemistry, Principles and Applications; Taylor &amp; Francis Group ,2010.</del></p> <p><del>D. Meyers, Surfaces, Interfaces and Colloids, Principles and Applications; John Wiley &amp; Sons, Inc. 1999. 2<sup>nd</sup> edition.</del></p> <p><del>E. D. Shchukin, A. V. Pertsov, E. A. Amelina, A. S. Zolotarev, Studies in Interface Science, Colloid and Surface Chemistry; Elsevier, 2001.</del></p> <p><del>D. J. Shaw, Introduction to Colloid and Surface Chemistry, 4<sup>th</sup> Ed Elsevier, 1992.</del></p> <p><del>F. Caruso, Colloids and Colloid Assemblies, Wiley-VCH, 2004</del></p> <p><del>V. Lesnyak, M. Yarema, S. Mizoguchi, Colloidal Semiconductor Nanocrystals: Synthesis, Properties and Applications, Frontiers Media SA, 2020.</del></p>
<p><b>Course Outcome:</b></p>	<ol style="list-style-type: none"> <li>1. Students will be able to explain various fundamental and core concepts of colloid chemistry.</li> <li>2. Students should be in a position to apply the knowledge of colloidal chemistry for their dissertation and research work</li> <li>3. Students should be in a position to apply these concepts during the lab course in physical chemistry.</li> <li>4. Students will understand applications of colloids.</li> </ol>



**Name of the Programme:** M.Sc. Part-II (Chemistry)

**Course Code:** CHC-600      **Title of the course:** Research Methodology and instrumental techniques-I

**Number of Credits:** 4

**Effective from AY:** 2023-24

<b>Prerequisites for the course:</b>	Students should have studied chemistry courses at MSc-I level.	
<b>Course Objective:</b>	<ol style="list-style-type: none"><li>1. To introduce various aspects of research methodology.</li><li>2. To provide understanding ethics &amp; scientific conduct.</li><li>3. To introduce academic writing.</li><li>4. To introduce databases used in chemistry.</li><li>5. To provide understanding and importance of lab safety.</li><li>6. To understand the usefulness of various instrumental techniques in characterization of chemical compounds.</li></ol>	
<b>Content</b>	<b>1. Introduction to Research Methodology</b> Research- meaning, objectives, motivation, types and methodology. Process- formulating the research problem; literature survey; developing the hypothesis and the research design; sample design and collection of the data; execution of the project; analysis of data; testing of hypothesis; generalizations and interpretation, and preparation of the report or presentation of the results & conclusions.	No of hours 5
	<b>2. Scientific conduct and ethics</b> Ethics: definition, nature of moral judgements and reactions, Ethics with respect to science and research. Intellectual honesty and research integrity. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP). Redundant publications: duplicate and overlapping publications. Selective reporting and misrepresentation of data.	5
	<b>3. Academic writing</b> Publication ethics: definition, introduction and importance Conflicts of interest Publication misconduct: definition, concept, problems that lead to unethical behaviour and vice versa Violation of publication ethics, authorship and contributorship Identification of publication misconduct, complaints and appeals Predatory publishers and journals	5

	<p><b>4. Data bases and research metrics</b>  Databases: 1. Indexing databases 2. Citation databases: Web of Science, Scopus, UGC-Care List etc.  Research Metrics: 1. Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score 2. Metrics: h-index, g index, i10 index etc</p>	3
	<p><b>5. Safety aspects in Chemistry</b>  Good laboratory practices.  Handling of various chemicals, solvents &amp; glassware.  Fires and fighting with fires.  Hazardous substances, classification and handling  Safety Data Sheet</p>	5
	<p><b>6. Softwares in Chemistry</b>  Data plotting  Structure Drawing  Reference management software</p>	7
	<p><b>7. Instrumental methods of analysis:</b>  Demonstration and/ or data analysis in following techniques:  Elemental analysis: CHNS analysis and AES  Infrared (IR), Raman, Ultraviolet-Visible (UV-Vis)  Nuclear magnetic resonance (<math>^1\text{H}</math>, <math>^{13}\text{C}</math>)  Chromatographic techniques: HPLC, GC,  Hyphenated Techniques: LC-MS &amp; GC-MS,  Diffraction methods: XRD  Thermal analysis: DSC  Microscopy: SEM, TEM  Methods for determination of magnetic &amp; dielectric properties.  Cyclic voltammetry</p>	30
<b>Pedagogy</b>	Mainly lectures/recorded video lectures/ tutorials, discussions, seminars, internal exams/ assignments, / demonstration/ self-study or a combination of some of these. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
<b>References / Readings</b>	<ol style="list-style-type: none"> <li>1. C. R. Kothari, Research Methodology: Methods &amp; Techniques, New Age International Pvt. Ltd., 2004.</li> <li>2. Bird, Philosophy of Science, Routledge, 2006.</li> <li>3. M. Coghill &amp; L. R. Garson, The ACS Style Guide: Effective Communication of Scientific Information, American Chemical Society Washington, DC &amp; OXFORD University Press New York, 2006.</li> <li>4. Y. K. Singh, Fundamentals of Research Methodology &amp; Statistics, New Age International Pvt. Ltd., 2006.</li> <li>5. National Research Council, Prudent practices in the laboratory: handling and management of chemical hazards, The National</li> </ol>	

	<p>Academies Press, USA, 2011.</p> <ol style="list-style-type: none"> <li>6. B. S. Furniss, A. J. Hannaford, P. W. G. Smith &amp; A. R. Tatchell, Vogel's Text book of Practical Organic Chemistry, 5th Ed.; Longmann, 1989</li> <li>7. E. A. V. Ebsworth, D. W. H. Rankin &amp; S. Craddock, Structural Methods in Inorganic Chemistry, Blackwell Scientific Publishers. 1986.</li> <li>8. R. S. Drago, Physical Methods in Chemistry, 2nd Ed. W. B. Saunders Co. Ltd. 2016</li> <li>9. R. M. Silverstein, F. X. Webster; Spectrometric identification of Organic Compounds; 6th Ed, Wiley, 2011.</li> <li>10. J. Mendham, R. C. Denny, J. D. Barnes &amp; M. Thomas, Vogel's Textbook of Quantitative Chemical Analysis, 6th Ed.; Pearson Education Asia, 2002.</li> <li>11. H. V. Keer, Principles of the Solid State, 1st Ed. New Age International (P) Ltd., 2005.</li> <li>12. G. D. Christian, Analytical Chemistry, 6th Ed.; Wiley, 2004.</li> <li>13. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamentals of Analytical Chemistry, 9th Ed.; Cengage learning.</li> <li>14. Skoog, F. J. Holler, S. R. Crouch, Principles of Instrumental Analysis, 7th Ed.; Cengage learning.</li> <li>15. P. G. Lampman, G. Kriz and J. Vyvyan, Introduction to Organic Spectroscopy, 5th Ed.; Cengage Learning, 2015.</li> <li>16. N. Elgrishi, K. J. Rountree, B. D. McCarthy, E. S. Rountree, T. T. Eisenhart, and J. L. Dempsey, A Practical Beginner's Guide to Cyclic Voltammetry, J. Chem. Educ. ACS, 2018, 95, 197–206.</li> <li>17. V. Rajaraman, Computer Programming in Fortran 90 And 95, PHI Learning Pvt. Ltd., 2013.</li> <li>18. Szabo, N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Publications, Inc. Mineola, 1989.</li> </ol>
<p><b>Course Outcome:</b></p>	<ol style="list-style-type: none"> <li>1. Students will be able to apply research methodology concepts.</li> <li>2. Students will be able to apply computer technology to solve their research problems in chemistry.</li> <li>3. Students will know in advance the safety precautions to be taken in the chemical lab.</li> <li>4. Students will gain fundamental knowledge on characterization techniques.</li> </ol>

**Name of the Programme:** M.Sc. Part-II (Chemistry)

**Course Code:** CHC-601      **Title of the course:** Research Methodology and instrumental techniques-II

**Number of Credits:** 4

**Effective from AY:** 2023-24

<b>Prerequisites for the course:</b>	Students should have studied chemistry courses at MSc-I.	
<b>Course Objective:</b>	1. To introduce various aspects of research methodology. 2. To provide understanding ethics & scientific conduct. 3. To introduce academic writing. 4. To introduce databases used in chemistry. 5. To provide understanding and importance of lab safety. 6. To understand the usefulness of various instrumental techniques in characterization of chemical compounds.	
<b>Content</b>	<b>1. Research Methodology, Scientific conduct, ethics &amp; academic writing</b> Research- meaning, objectives, motivation, types and methodology. Process- formulating the research problem; literature survey; developing the hypothesis and the research design; sample design and collection of the data; execution of the project; analysis of data; testing of hypothesis; generalizations and interpretation, and preparation of the report or presentation of the results & conclusions. Ethics: definition, nature of moral judgements and reactions, Ethics with respect to science and research. Intellectual honesty and research integrity. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP). Redundant publications: duplicate and overlapping publications. Selective reporting and misrepresentation of data. Publication ethics: definition, introduction and importance Conflicts of interest Publication misconduct: definition, concept, problems that lead to unethical behaviour and vice versa Violation of publication ethics, authorship and contributorship Identification of publication misconduct, complaints and appeals Predatory publishers and journals	No of hours  15
	<b>2. Softwares in chemistry, Data bases and Research metrics</b>	10

	<p>Data plotting using GNU plot; Structure Drawing using ChemSketch; Reference management software such as Mendeley and Zotero.</p> <p>Databases: Indexing databases, Citation databases: Web of Science, Scopus, UGC-Care List, Scimago etc.</p> <p>Research Metrics: Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score; Metrics: h-index, g-index, i10-index etc</p> <p>Molecular Docking software</p>	
	<p><b>3. Safety practices in Chemical research</b></p> <p>Introduction to lab safety.</p> <p>Handling of various chemicals, solvents &amp; glassware.</p> <p>Fires and fighting with fires.</p> <p>Hazardous substances, classification and handling</p> <p>Safety Data Sheet</p>	5
	<p><b>4. Instrumental methods</b></p> <p>UV-Visible spectroscopy in elucidation of mechanisms of C-H activation reactions, epoxidation etc by transition metal catalyst.</p> <p>Understanding water oxidation reaction using Cyclic voltammetry (CV) &amp; Linear Sweep voltammetry (LSV)</p> <p>Determining capacity of supercapacitors using Galvanostatic Charge-Discharge (GCD)</p> <p>Electrochemical Impedance Spectroscopy (EIS)</p> <p>Resonance Raman and isotope labelling studies.</p> <p>Infrared (IR) spectroscopy applications</p> <p><sup>1</sup>H, <sup>13</sup>C- NMR spectroscopy and applications</p> <p>Selected chromatographic techniques such as HPLC, GC.</p> <p>Hyphenated Techniques/applications: LC-MS, GC-MS, LC-NMR-MS, GC-IR, ICP-MS</p> <p>Diffraction methods: High temperature XRD</p> <p>Thermal analysis: TG/DTA/DSC</p> <p>Microscopy: Fe-SEM, HR-TEM</p> <p>Methods for determination Ms, Mr, Hc, Tc, <math>\epsilon^1</math> and Tan<math>\delta</math>.</p> <p>Potentiometry</p>	30
<b>Pedagogy</b>	<p>Mainly lectures/recorded video lectures/ tutorials, discussions, seminars, internal exams/ assignments, / demonstration/ self-study or a combination of some of these. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.</p>	
<b>References / Readings</b>	<ol style="list-style-type: none"> <li>1. C. R. Kothari, Research Methodology: Methods &amp; Techniques, New Age International Pvt. Ltd., 2004.</li> <li>2. Bird, Philosophy of Science, Routledge, 2006.</li> <li>3. M. Coghill &amp; L. R. Garson, The ACS Style Guide: Effective Communication of Scientific Information, American Chemical Society Washington, DC &amp; OXFORD University Press New York,</li> </ol>	

	<p>2006.</p> <ol style="list-style-type: none"> <li>4. Y. K. Singh, Fundamentals of Research Methodology &amp; Statistics, New Age International Pvt. Ltd., 2006.</li> <li>5. National Research Council, Prudent practices in the laboratory: handling and management of chemical hazards, The National Academies Press, USA, 2011.</li> <li>6. B. S. Furniss, A. J. Hannaford, P. W. G. Smith &amp; A. R. Tatchell, Vogel's Text book of Practical Organic Chemistry, 5th Ed.; Longmann, 1989</li> <li>7. E. A. V. Ebsworth, D. W. H. Rankin &amp; S. Craddock, Structural Methods in Inorganic Chemistry, Blackwell Scientific Publishers. 1986.</li> <li>8. R. S. Drago, Physical Methods in Chemistry, 2nd Ed. W. B. Saunders Co. Ltd. 2016</li> <li>9. R. M. Silverstein, F. X. Webster; Spectrometric identification of Organic Compounds; 6th Ed, Wiley, 2011.</li> <li>10. J. Mendham, R. C. Denny, J. D. Barnes &amp; M. Thomas, Vogel's Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> Ed.; Pearson Education Asia, 2002.</li> <li>11. H. V. Keer, Principles of the Solid State, 1st Ed. New Age International (P) Ltd., 2005.</li> <li>12. G. D. Christian, Analytical Chemistry, 6th Ed.; Wiley, 2004.</li> <li>13. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamentals of Analytical Chemistry, 9th Ed.; Cengage learning.</li> <li>14. Skoog, F. J. Holler, S. R. Crouch, Principles of Instrumental Analysis, 7th Ed.; Cengage learning.</li> <li>15. Pavia, G. Lampman, G. Kriz and J. Vyvyan, Introduction to Organic Spectroscopy, 5th Ed.; Cengage Learning, 2015.</li> <li>16. N. Elgrishi, K. J. Rountree, B. D. McCarthy, E. S. Rountree, T. T. Eisenhart, and J. L. Dempsey, A Practical Beginner's Guide to Cyclic Voltammetry, J. Chem. Educ. ACS, 2018, 95, 197–206.</li> <li>17. V. Rajaraman, Computer Programming in Fortran 90 And 95, PHI Learning Pvt. Ltd., 2013.</li> <li>18. Attila Szabo, Neil S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Publications, Inc. Mineola, 1989.</li> <li>19. Leach, Molecular Modelling, Principles and applications, Longman, 1998.</li> <li>20. W. Nam et al, Dioxygen activation by Metalloenzymes &amp; models, Accounts of Chemical Research, 2007, Volume 40 &amp; references cited therein.</li> </ol>
<p><b>Course Outcome:</b></p>	<ol style="list-style-type: none"> <li>1. Students will be familiar with research methodology concepts.</li> <li>2. Students will be able to apply computer technology to solve their research problems in chemistry.</li> <li>3. Students will know in advance the safety precautions to be taken in the chemical lab.</li> <li>4. Students will gain fundamental knowledge on characterization techniques.</li> </ol>

**Name of the Programme:** M.Sc. Part-II (Chemistry)

**Course Code:** CHC-651      **Title of the course:** Discipline Specific Dissertation

**Number of Credits:** 16

**Effective from AY:** 2023-24

<b>Prerequisites for the course:</b>	Students should have studied chemistry courses at MSc-I level.	
<b>Course Objective:</b>	To develop the skills of preparing and conducting independent research.	
<b>Content</b>	As per OA-35	No of Hours 480
<b>Pedagogy:</b>	Dissertation carried out individually by each student throughout the academic year.	
<b>References / Readings:</b>	As required for the development of review and methodology.	
<b>Course Outcome:</b>	Students will be able to understand and apply the tools and techniques of chemistry in conducting independent research.	