

## Courses of Study

**Programme: M Phil (Applied Chemistry) Duration: 1 year**

<b>I – Semester Course</b>			
<b>Course No.</b>	<b>Course</b>	<b>LTP</b>	<b>Credit hr.</b>
<b>Theory papers: Core courses</b>			
AMD61141 ACD61156	Computer Programming and Computer Applications in Chemistry Part A. Computer Programming Part B. Computer Applications in Chemistry	2-0-0 2-0-0	8
ACC61157	Instrumental Techniques in Chemistry –I	3-0-0	6
ACC61158	Instrumental Techniques in Chemistry – II	3-0-0	6
<b>Elective courses (any two of the courses listed below)</b>			
ACE61159	Environmental Chemistry	3-0-0	6
ACE61160	Ceramic Materials	3-0-0	6
ACE61161	Science of Corrosion and Corrosion Control	3-0-0	6
ACE61162	Polymer Chemistry	3-0-0	6
ACE61163	Industrial Chemistry	3-0-0	6
<b>Practical courses: Core courses</b>			
AMD61241 ACD61256	Computer Programming and Computer Applications in Chemistry (Practical) Part A. Computer Programming Part B. Computer Applications in Chemistry	0 0 2/2 0 0 2/2	1 1
ACC61257	Chemistry Practical –I	0-0-3	3
ACC61258	Chemistry Practical –II	0-0-3	3
<b>Seminar/ Dissertation/ Viva-voce</b>			
ACC61401	Seminar – I	0-0-0	6
<b>Total</b>		<b>16 0 8</b>	<b>46</b>

<b>II Semester</b>			
ACC 62402	Seminar – II	0-0-0	6
ACC 62401	Dissertation	0-0-0	28
ACC 62501	Viva Voce	0-0-0	12
<b>Total</b>			<b>46</b>

**SYLLABUS (THEORY)****Computer Programming and Computer Applications in Chemistry****AM D 6 1 1 4 1 (200) Part A. Computer Programming**

OOPs : Basic concepts of OOPs; C<sup>++</sup> preliminaries, data types, arrays, functions, classes and objects, constructors and destructors, function overloading, operator overloading and Type conversions; inheritance, pointers polymorphism, console oriented I/O operations, file management, templates, exception handling.

JAVA : introduction to JAVA

**AC D 6 1 1 5 6 (200) Part B. Computer Applications in Chemistry**

Programs for simple formulas – mean free path of gas molecules, effusion velocity of gas, heat transfer according to second Fourier law, partition function. Compilation of table: mean values and standard deviation. Monte Carlo integration. Simulation of copolymerisation reaction. Monte Carlo calculation of first order kinetics. Linear Regression, least square method. Calibration curve using Gauss Jordan method. Non-linear regression applications in adsorption. Introduction to computer aided organic synthesis.

**AC C 6 1 1 5 7 (300) Instrumental Techniques in Chemistry -I**

Nuclear Magnetic Resonance: General introduction, principle, instrumentation, (CW&FT) chemical shifts, spin-spin interaction, shielding mechanism, chemical exchange, First order Spectra, virtual coupling, Karplus Curvature variation constants with dihedral angles, contact shift reagents, application of <sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F & <sup>31</sup>P NMR.

UV- Visible Spectroscopy: Principle, instrumentation, Electronic excitations, common chromophore groups. Application of UV to conjugate dienes, polymers,  $\alpha$ ,  $\beta$ - unsaturated carbonyl compounds, Benzene and its substituted derivatives. Heterocycles, cis & trans-isomers.

Mass Spectroscopy: Basic Principles, Instrumentation, Isotope, abundance, metastable ions, Fragmentation Process, application of mass spectroscopy to various organic compounds (GC-MS and LC-MS)

XRF and X-ray spectroscopy: Principles and applications of x-ray spectroscopy, X-ray fluorescence, Energy dispersive and wavelength dispersive x-ray spectroscopy.

IR spectroscopy: Introduction & Theory, Molecular vibration, vibrational frequency, number of fundamental vibrations. Factors influencing vibrational frequencies. Sampling techniques. Application of IR spectroscopy in organic and in inorganic chemistry.

Atomic Absorption Spectroscopy: Principle, Instrumentation and application.

### **AC C 6 1 1 5 8(300) Instrumental Techniques in Chemistry-II**

Thermo Analytical Method: Thermo gravimetric analysis, Differential thermal analysis (DTA), DSC and DMA. Thermometric titrations, thermal methods in quantitative analysis.

Electro analytical Techniques: Introduction, classification of methods, Potentiometric method potentiometric titrations, titration in nonaqueous solvents, ion selective electrode. Voltametry and related techniques- Diffusion limiting current, dropping mercury electrode (DME) voltage- scanning polarography, shape of the polarographic wave, qualitative and quantitative analysis, organic polarography, amperometric titrations, chronopotentiometry. Conductimetric Method- Instrumentation, analytical applications, conductometric titrations, high Frequency titrations. Electro-deposition methods- controlled potential electrolysis, coulometry, coulometric titrations, stripping analysis. Electrochromatography- chromatography, classification of chromatographic method, development of chromatogram, principles of electrophoresis, apparatus and methodology, analytical applications of electrochromatography, reverse osmosis, electro dialysis.

GC and HPLC: Theory, instrumentation, working applications, programmed temperature gasflowchromatography.

### **AC E 6 1 1 5 9 (300) Environmental Chemistry**

Atmosphere: Composition & structure of atmosphere, particles, ions and radicals in the atmosphere, stratospheric ozone depletion.

Air Pollution: Air Pollutants, e.g. carbon monoxide, nitrogen oxides, hydrocarbons, oxides of sulfur, photochemical smog, acid rain & particulates. Air quality standards and sampling monitoring of CO, NO<sub>x</sub>, and SO<sub>2</sub>. Automobile pollution. Effect of pollutants.

Hydrosphere : Water resources, hydrologic cycle. Complexation in natural and waste water. Micro organism.

Water Chemistry: Principles and applications of aqueous chemistry and unique properties of water. Water quality parameters and standards. Acid mine drainage, heavy metal pollution, eutrophication, soap and detergents, pesticides, nitrates, fluorides- effect and abatement.

Lithosphere : Composition, inorganic & organic compounds in soil, Acid-base and ion exchange reaction in soil, micro and macro nutrients, nitrogen pathways and NPK in soil, waste classification & disposal.

**AC E 6 1 1 6 0 (300) Ceramic Materials**

Ceramic materials, various ceramic systems, metal, pore, glass, ceramic microstructure. Crystal chemistry of ceramic materials, ceramic processing, Microstructure and compositional characterization.

Fibre reinforced ceramic systems.

Ceramic matrix composites: Particulate reinforced, continuous fibre, chopper fibre, whisker reinforced; fabrication and properties. Applications of composites.

Advanced ceramic materials: Preparation and properties. Nano-structured materials.

Mechanical and thermal properties of ceramic materials, Mechanical behaviour of materials, based on atomic and microstructural consideration and thermal application.

Electrical and magnetic behaviour of ceramic materials. Properties and production of ceramic materials used for dielectric, optical, semiconductor, ion conductor & magnetic applications.

Theory of vitreous state, structure of glasses, nucleation theory, control of diversification, composition, structure-property relationship. Ceramic processing: Power processing rules, sol-gel techniques, desiccations.

Refractories: Mineralogy, manufacture and service characteristics of refractory materials. Use of refractories in metallurgical and ceramic industries.

**AC E 6 1 1 6 1 (300) Science of Corrosion and Corrosion Control.**

Corrosion, theories of corrosion. Kinetics of corrosion, Evans' diagram, thermodynamics of corrosion-Pourbaix diagram. Forms of corrosion.

Corrosion prevention: modification of materials, corrosion inhibitors, protective coatings, cathodic and anodic protection.

Corrosion testing techniques: Evaluation of corrosion effect- XRD, ESCA, FTIR and surface techniques

Corrosion in industries with special reference to oil and mining industries.

**AC E 6 1 1 6 2 (300) Polymer Chemistry**

Introduction: Basic concepts molecular forces and chemical bonding and analysis

Characterization of Polymers: Fractionation of polymers by solubility, Gel permeation chromatography, Size exclusion chromatography. Molecular weight distribution and analysis, colligative properties measurement, light scattering, viscosity.

Structure and properties of polymers: Polymer structure physical properties relationship and polymer utilization. IR spectroscopic, XRD, NMR, ESR, Thermo-analytical and Microscopic techniques of analysis.

Polymerization reaction: Synthesis of polymer precursors, Polymer additives. Properties of some commercial polymers

**AC E 6 1 1 6 3 (300) Industrial Chemistry**

Petrochemicals: Introduction. Classification of petrochemicals. Manufacture of some common petrochemicals.

Explosives: Characteristics of explosives, classification of explosives- primary & secondary explosives, preparation and application of some commercial explosives.

Cement: Types and composition of cements, raw material, manufacturing. Chemistry of setting of cement. Various additives used. Reinforced cement concrete. High performance concrete.

Dust Suppressant: Chemistry and source of dust. Dust suppressants.

Paints and Pigment: Pigments-characterization and types, properties. Paints-classification, properties and applications of paints. Manufacture of paints.

**SYLLABUS (PRACTICAL)****AM D 6 1 2 4 1 (002/2) Part A. Computer Programming**

Execution of programs using the following:

Control Structures, Arrays, Function subroutine and Subroutine subprogram, File Processing

**AC D 6 1 2 5 6 (002/2) Part B. Computer Applications in Chemistry**

Computer programs on potentiometric titration simulations, regression analysis, multicomponent analysis.

**AC C 6 1 2 5 7 (003) Chemistry Practical – I**

Estimation of elements by AAS and by UV-Vis spectroscopy. NMR interpretation of a given sample, qualitative analysis of pharmaceuticals. Sample preparation for FTIR spectroscopy. Purity determination of organic samples by FTIR and DSC.

**AC C 6 1 2 5 8 (003) Chemistry Practical –II**

Practical will be conducted on Identification and separation of known samples by TLC techniques and conductometric titration of a given sample. Analysis using Thermal methods, SEM and EDX analysis. BOD, COD and DO of effluents