

AWADHESH PRATAP SINGH UNIVERSITY,

REWA

Structure of Syllabus for Ph.D. Course Work (Chemistry) 2018-19 Onwards
(As per Ordinance No. 11 Doctor of Philosophy)

Paper Code	Name of Theory Papers	Credits	Maximum Marks (Theory+ Internal Assessment)	Minimum Passing Marks
Ph.D. 101	RESEARCH METHODOLOGY	✓ 4	100 (80+20)	55
Ph.D. 102	REVIEW OF PUBLISHED RESEARCH IN THE RELEVANT FIELD	3	100	55
Ph.D. 103	COMPUTER APPLICATIONS	✓ 3	100 (80+20)	55
Ph.D. 104	SPECIALIZATION SUBJECTS Techniques and Theoretical approach	✓ 3	100 (80+20)	55
Ph.D. 105	COMPREHENSIVE VIVA-VOCE	3	100	55
TOTAL		16 Credits		

Ph. D. (Chemistry)
Paper- Ph.D. 101 Research Methodology

Time: 03 Hours

Theory Paper : Max. Marks-80
Internal Assessment : Max. Marks-20
Minimum Pass Marks-55

The paper setter is required to set in all **Eight** questions, out of which only **four** questions are to be attempted by the students. All questions will be of equal marks. Two questions are to be set from each unit. The students are required to attempt at least one question from each unit.

Unit-I: Introduction

A. Basic steps for doing research

Literature survey, Investigation, Analysis of data, Preparation of manuscript, Publication of research work, Example of a research paper

B. Error Analysis

Random and systematic errors, Significant figures, Approximate numbers, Rounding off numbers, Presentation of errors, Index of accuracy, Error formulas

Unit-II: Arrangement of Data

Sampling, Arrangement of data, Arithmetic mean, Median, Variance, Standard deviation, Probability distribution, Correlation, Regression

Unit-III: Chi-square Tests and Analysis of Variance

Chi-square distribution, Chi-square test for comparing variance, Chi-square test ANOVA technique, One-way ANOVA technique, Two-way ANOVA technique, ANOVA in a Latin square design

Unit-IV: Separation Techniques

Introduction, Oxidation-Reduction Processes, Complexation, Solvent Extraction, Volatilization and Distillation, Electrodeposition, Chromatography, Precipitation and Coprecipitation

Books:

1. Research Methodology, S. Chandra and M. K. Sharma, Narosa Publishing House.
2. Computers and Common Sence, R. Hunt and J. Shelley, Prentice Hall.

Ph. D. (Chemistry)
Paper- Ph.D. 103 Computer Applications

Time: 03 Hours

Theory Paper : Max. Marks: 80
Internal Assessment : Max. Marks: 20
Minimum Pass Marks: 55

The paper setter is required to set in all Eight questions, out of which only four questions are to be attempted by the students. All questions will be of equal marks. Two questions are to be set from each unit. The students are required to attempt at least one question from each unit.

Unit-I: Networking and search Internet

Historical background, Need & Advantage of computer network, anatomy of computers and their classification, Type of computer network, LAN, MAN, WAN Basic HW & SW requirement for networking, Preliminary introduce of modem, can card, various communication media, HUB, Switches routers and gateway, Wireless network, The internet its application, WWW creation of web sites, searching and assessing information from web, using ftp & telnet.

Unit-II: Computers applications in Inorganic Chemistry

Shapes of ions and molecules using VSEPR theory
Doppler shift and recoil velocity from Mossbauer data
Concentration of complexes using Beer's Lambert's law
Bonding energy of a nucleus
d-orbital splitting in octahedral field
Solubility of sparingly soluble salt

Unit-III: Computers applications in Organic Chemistry

Synthesis of Organic compounds
Dipole moments of disubstituted benzene
Resonance energy for organic conjugated systems (Heat of combustion)
Isoelectric point of amino acids
 ^{13}C chemical shift in organic compounds
Woodward Hoffman rules in pericyclic reaction

Unit-IV: Computers applications in Physical Chemistry

Determination of constants, a, b, g and axial ratio a': b': c' for crystals
Delocalization energy for butadiene using Group theory
Symmetry numbers for molecules using data on symmetry operations
Character table for C_{3v} point group
Wave numbers of stokes and anti-stokes lines
Parameters from NMR and ESR data

Books:

3. Computers in Chemistry, K V Raman; Tata McGraw-Hill Publishing.
4. Computers and Common Sence, R. Hunt and J. Shelley, Prentice Hall.
5. Computational Chemistry, A. C. Norris.
6. Internet Technology, V. K. Jain, DOEACC.
7. Computer Programming in FORTRAN IV, V. Rajaram, Prentice Hall.

Ph. D. (Chemistry)

Paper- Ph.D. 104 Specialization : Techniques and Theoretical approach
Time: 03 Hours

Theory Paper : Max. Marks-80
Internal Assessment : Max. Marks-20
Minimum Pass Marks-55

The paper setter is required to set in all Eight questions, out of which only four questions are to be attempted by the students. All questions will be of equal marks. Two questions are to be set from each unit. The students are required to attempt at least one question from each unit.

Unit-I: Voltammetry and Polarography

Fundamental of Voltammetry, Conventional or d.c. voltammetry, Conventional or d.c. polarography, Theoretical principal, Complex Ion, Quantitative techniques, The effect of oxygen, Simple polarography and classical d. c. polarography, The three electrode polarograph: potentiostatic control, Modified voltammetry. Principal and instrumentation, Brief description of polarographic measurement, Current voltage relationship, Polarograms interpretation of polarographic waves. Equation for the polarographic waves, Half wave potential and its importance, The kinetic and catalytic currents, Polarographic cell, the dropping mercury electrode, Advantages of DME, Limitations of DME, The capillary and its care, Condition for performing polarographic determinations, Advantages of polarography, Application of polarography, Quantitative analysis, Qualitative analysis, Inorganic polarographic analysis, Organic polarographic analysis, Stationary electrode (slow linear scan) polarography, Cathode ray (rapid linear scan) polarography. Anodic stripping (inverse polarography), Alternating current polarography, Chronopotentiometry, Instrumentation and procedure, Application.

Unit-II: Molecular structure determination using NMR, ESR and NQR.

NMR- Introduction, Theory, The chemical shift, Coupling of magnetic nuclei, Instrumentation, Sample preparation, Experimental determination (Ethanol content of an alcoholic liquor & Ethanol content of a beer by standard addition). ESR- The technique, epr parameters, epr spectral analysis of some organic and inorganic compounds especially transition metal complexes. The g-value, Hyperfine structure. NQR- Theory, Principle, Instrumentation and application.

Unit-III: Molecular structure determination

A. Using diffraction techniques (X-ray, neutron & electron)

Introduction, Particles and waves Crystal lattice (Crystal morphology, Lattice and unit cells), X-ray diffraction (The powder method, Symmetric absence, Fourier synthesis) Information from X-ray analysis, Neutron diffraction & electron diffraction- Basic principle, Instrumentation and application in chemistry

B. Using Photoelectron spectroscopy

The techniques, UPS, XPS and Basic principal and instrumentation of ESCA (electron spectroscopy for chemical analysis) & analysis of different photoelectron spectra (HBr, NaN_3 & Moon dust).

Unit-IV: Topological parameters

Topology

What are topological parameters?, Distance matrices of chain and classic graphs, Calculation of Wiener index, S_z index, Path number, PI index, Balaban index, in case of benzene, quinoline, acridine, pyridine and their derivatives

QSAR