

**School of Studies in Chemistry and Biochemistry
Vikram University, Ujjain**



According to Ph. D. Ordinance No. 11NEW

**Course Work
(Syllabus)
Ph. D. (Chemistry)**

Session 2019-20

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**School of Studies in Chemistry and Biochemistry
Vikram University, Ujjain**

**According to Ph. D. Ordinance No. 11NEW
Course Work**

Scheme & Syllabus for Ph. D. (Chemistry)

First Semester

Session 2019-20

Scheme of Papers/ Examination

Paper	Titles of Paper	Maximum Marks			Credits
		End-Semester Examination	CCE	Total	
I	Research Methodology	60	40	100	4
II	Computer Applications	60	40	100	3
III	Spectral and Analytical Chemistry	60	40	100	3
	Review of published research in relevant field	60 (written report)	40 (oral presentation)	100	3
	Comprehensive Viva-voce			100	3
Total				500	16

Note:

1. If a student obtains F or Ab Grade in a course/subject, he/she will be treated to have failed in that course. He/she have to reappear in the examinations of the course as and when conducted or arranged by the UTD in the next semester. Marks obtained earlier in continuous assessment may be carried forward and added to the marks obtained in repeat end semester examination to decide the grade in the repeat course. The student has to pay the prescribed fee for repeating the course. If he/she further fails in the course, he/she shall not be given another chance and he/she shall be out of the Ph. D. programme. No student shall be allowed to repeat the course to improve the grade of he/she passes the course.
2. The candidate has to obtain a minimum of 55% of marks or its equivalent grade points in aggregate in the course work in order to be eligible to continue in the Ph. D. programme.

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Course Work
Syllabus for Ph. D. (Chemistry)
First Semester

Paper I

(100 Marks/4 Credits)

Research Methodology

Unit I

Introduction to research methodology, design and implementation of research methods, types and steps in research, Objectives of research, Techniques of research formulating, reviewing the literature.

Mode of approach of actual investigation, Drawing inferences from data- Qualitative and Quantitative research approaches, Assessing the status of the problem, Characteristics and components of research problem.

Unit II

Basic concepts of research Paper/Thesis writing and report generation, Writing research abstract, summary, Introduction, review of literature, materials and methods, presenting the results, writing the discussions and citing the references, Types of research studies and research methods, Data collection and data analysis

Writing scientific report: Planning, preparation, draft, revision and refining; writing project proposal to funding agency

Unit III

Testing of Hypothesis: Meaning, Basic concepts, Flow diagram, Power of a hypothesis test, Important Non-Parametric tests: Sign, Run, Kruskal-Wallis tests and Mann-Whitney test, Important parametric tests, Hypothesis Testing of Means, Comparing Two related samples, Testing of Proportion, Difference between proportions, Comparing variance to hypothesized population variance, Chi-square tests-ANOVA-One way and Two way, Equality of

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variances of two normal populations, hypothesis testing of Correlation coefficients, Limitations of Tests of hypothesis.

Unit IV

Ethical Issues : Code of Ethics in Research, Ethics and research process, Importance of ethics in research, Ethical committees, Commercialization, copy right, royalty, intellectual property and patent law, track related aspects of intellectual property rights, Reproduction of published material, Plagiarism, citation and acknowledgement, reproducibility and accountability, Editing

Unit V

Sampling – introduction, definitions, theory of sampling, techniques of sampling, central limit theorem, Sandler's A test, statistical criteria of good sampling and required size, stratified sampling vs random sampling, minimization of variance in stratified sampling, transmission and storage of samples, Concept of standard error.

Reference Books

1. The art of Scientific Writing – H.F. Ebel, C. Bliefert and W.E. Russey , WILEY-VCH Verlag GmbH & Co, K G a A.Wecnhcim 2nd Edn(2004)
2. Tests, Measurements and Research Methods in Behavioral Sciences : A. K.Singh.
3. Statistics for Analytical chemists, First Ed., By R Caulcutt and R Boddy, Chapman & Hall, (1983).
4. *Thesis and Assignment Writing*, J. Anderson, B.H. Dursten and M. Poole, Wiley Eastern, (1977).
5. *Research Methodology*, C.R.Kothari, New Age International Publishers, (2004).
6. *Fundamental of Research Methodology and Statistics*, Yogesh Kumar Singh, New Age International Publishers, (2006).
7. Fundamentals of Mathematical Statistics, Gupta,S.C. and Kapoor, V.K. (2002). Educational Publishers, New Delhi.
8. An Introduction to Research Methodology, RBSA Publishers. Garg, B. L. Karadia, R. Agarwal, F. and Agarwal, U.K.(2002)

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Course Work
Syllabus for Ph. D. (Chemistry)
First Semester

Paper II

(100 Marks/3 Credits)

Computer Applications

Unit I

Introduction to computers- history of development of computers Main frame mini, micro and super computer systems-computer hard ware CPU, input, output devices, auxiliary storage devices, interpreter, compiler, machine language, assembly language, high level languages

Unit II

Introductory Operatives-Package, MS Word: word basics, formatting text and documents, introduction to mail merge & macros. MS Excel: Excel basics, rearranging worksheets, working with charts and graphs, using worksheet as databases, Use formulas and functions, MS PowerPoint : PowerPoint basics, creating presentation MS Access: Database creation, screen/form design, generation using wizard, Preparation of a document, Editing of a document, Preparing a scientific manuscripts, Features of Acrobat Reader.

Unit III

Programming with C: Character Set, Identifiers, Keywords, Variables, Character Strings, Qualifiers, Typecasting, Constants, Operator and Expression, Operator Precedence and Associativity, Input-Output Statements. Control Statements: if, if-else, nested if, if-else ladder, switch Statements, Loops: for, while do-while, break and continue statement, Arrays, Strings.

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Unit IV

Literature Searching: On-line searching, Database, Scifinder, Scopus, Locating research article, Citation Index, Impact Factor

Computer Software in Chemistry: Instrument Control, Instrument Maintenance and Calibration system, Graphical Display of Data and Molecular Structures, Chem Office, Chemdraw, Chemistry 4-D Draw Standard.

Unit V

Introduction to Internet and its applications: web browsers – World Wide Web, Search Engines, e-journals, literature Survey, Popular journals and websites, literature searching and collection using e-journals.

Preparing presentations:

- i) Research papers: Using word processing software – MS Word, Drawing graphs and diagrams – Excel. Paper writing for International Journals, Process for online submission
- ii) Seminar presentations – Power point for oral and poster presentations

Reference Books

1. Programing in ANSI C. Balagurusamy, E.(2012):Tata McGraw Hill.
2. Introduction to Statistics with R, Second Edition, Springer. Dalgaard, P. (2008)
3. Let Us C, BPS Publication. Kanetkar, Y. (2008)
4. Fundamental of computers. Rajaraman, V.(2003). PHI Learning Pvt. Ltd.
5. Computer Fundamentals, BPS Publication. Sinha, P.K. and Sinha, P.(2007)
6. An Introduction to R. Venables, W.N. Smith, D. M. and R core Team.

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Course Work
Syllabus for Ph. D. (Chemistry)
First Semester

Paper III

(100 Marks/3 Credits)

Spectral and Analytical Chemistry

Unit I

IR and Raman spectroscopy, Instrumentation, preparation of samples and pellet making, Molecular vibrations, selection rules, force constant - band assignments, applications, organic structures, finger printing, identification of common functional groups, applications.

Effect of isotopic substitution on the vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment)

Raman spectroscopy: Stokes and anti-Stokes lines, Polarizability ellipsoids, Rotational and Vibrational Raman spectroscopy, Selection rules, Polarization of Raman lines, Applications of Raman Spectroscopy, Photo electron spectroscopy-principle and applications, Auger electron spectroscopy, electron spectra in chemical analysis.

UNIT II

NMR spectroscopy Bloch equations, the quantum mechanical description of the NMR experiment, transition probabilities, Fourier transform NMR, Relaxation effects, measurements of T1 and T2. Spectral simplification and determination of signs of coupling constants, elementary aspects of Solid State NMR.

¹H NMR spectroscopy, coupling constant, first order and second order splitting spin, spin splitting, dependence of J on dihedral angle, vicinal and geminal coupling constants, Karplus equation, long range coupling constants, influence of stereo chemical factors on chemical shift of protons, simplification of

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complex spectra, double resonance techniques, shift reagents, chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOH, NH, NH₂), an elementary treatment of NOE phenomenon, 2D technique (COSY, NOESY and ROSY)

¹³C NMR spectroscopy. Basic theory of FT NMR, Relaxation, broad band decoupling. Off resonance decoupling and chemical shift correlations (CH, CH₂, CH₃, =CH₂, =C, aromatic), NMR in medicine

UNIT III

UV Visible spectroscopy, Electronic excitation, origin of different bands, intensity of bands, selection rules - laws of photometry, correlation of electronic absorption with Molecular structure, chromophoric groups, conjugated systems, systems of extended conjugation, aromatic systems, empirical rules, experimental methods, photometric titrations.

Jablonskii diagram, Fluorescence and phosphorescence and factors affecting these, Calculation of excited state life-times from absorption data, Quenching of fluorescence, Stern-Volmer equation.

UNIT IV

Mass Spectrometry Principles, Instrumentation, Different ionizing techniques (EI, CI, FD, FAB, ESI, MALDI) - Various analysers (Magnetic sector, Quadrupole, Ion trap, ToF), Factors affecting fragmentation, ion analysis. Ion abundance, Analysis of mass spectrum, simple cleavage, β cleavage, allylic cleavage, benzylic cleavage, Factors affecting fragmentation pathways, McLafferty rearrangement, ortho effect, Fragmentation patterns of common organic compounds. Problems based on UV, IR, NMR and Mass spectral data.

UNIT V

Separation Methods: Theory and applications of separation methods in analytical chemistry, liquid-liquid extraction: Distribution coefficient, distribution ratio, solvent extraction of metals, multiple batch extractions,

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countercurrent distribution., multiple extractions solvent extraction, ion exchangers including liquid ion exchangers.

Introduction, fundamentals, principle, instrumentation and applications of gas chromatography, HPLC and other hyphenated Techniques: LC-MS, GC-MS, IC-MS, HP-TLC, and ICP-MS Spectroscopy

Reference Books

1. Spectrometric identification of organic compounds – R.M.Silverstein, G.C. Bassler and Morrill. John Wiley & Sons, New York 5th Edn (1991).
2. Physical methods in Inorganic chemistry – R. S.Drago Reinhold Pub.Corp.,(1965)
3. Physical methods in Organic Chemistry – Scharz. Oliver & Boyd,(1964)
4. Applications of absorption spectroscopy of organic compounds – J.Dyer.
5. Organic spectroscopy – W.Kemp. Macmillan, (1987)
6. An introduction to spectrometric methods for the identification of organic compounds Vol.I& II – F.Schlenk. Pergamon Press, Oxford (1970)
7. Introduction to spectroscopy – A guide for students of organic chemistry – D.L.Pavia,G.M.Lampman and G.S.Kniz Jr.
8. Instrumental methods of analysis – H.Willard, L.Merritt Jr.and A.Dean. 4th Edn(1996)
9. Fundamentals of analytical chemistry – D.A.Skoog and M.West.7th Edn, Saunders College Pub (1996)
10. Fundamentals of molecular spectroscopy – C.N.Banwell. 4th MC. Graw-Hill,(2008)
11. Basic principles of spectroscopy – R.Chang.
12. Spectroscopy of organic compounds – P.S Kalsi. New Age International 6th Edn (2009)
13. Practical Skills in Chemistry, J. R. Dean, A. M. Jones, D. Holmes, R. Reed, J. Weyers and A Jones, Pearson Education Ltd. [Prentice Hall] (2002)

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Course Work
Ph. D. (Chemistry)
Session 2019-20

	Marks
• Review of published research in relevant field	100
• Comprehensive Viva-voce	100

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