मौलाना आज़ाद नेशनल उर्दू यूनिवर्सिटी مولانا آزاد نیشنل اُردو یونیورسٹی
MAULANA AZAD NATIONAL URDU UNIVERSITY
(A Central University established by an Act of Parliament in 1998)
Gachibowli, Hyderabad – 500 032.
(Accredited "A" Grade by NAAC)

Section: Chemistry **School: School of Science**

Ph.D Chemistry

Ph.D in Chemistry Course Work Ist Semester		
Paper	**Paper code**	**Paper title**
1st	PHCH101CCT	Research Methodology
2nd	PHCH102CCT	Advanced Instrumentation
3rd	PHCH101DST	Synthesis and Reactivity of Natural Products
4th	PHCC104CCT	Research and Publication Ethics

Ph.D in Chemistry
(Syllabus of Paper -1)

Course Code **PHCH101CCT**
Course Title **Research Methodology**

Scheme of Instruction
Total Duration : **60Hrs**
Periods /Week : **4**
Credits : **4**
Instruction Mode : Lecture

Scheme of Examination
Maximum Score : **100**
Internal Evaluation : **30**
End Semester : **70**
Exam Duration : **3 Hrs**

Course Objectives: The main purpose of this course is to enhance student's Research and Technical skills. This course attempts to introduce the Approach towards Solution to Research problem, Publication of their Experimental Results, knowledge of different types of Chromatographic Techniques, Word processing operations and Presentation basics.

Course Outcomes:

Understanding of various Research Methodologies, Concepts of Chromatography and the Successful preparation of Research papers and Thesis

Unit	Course Content	Instruction Hours
1.	**Research** – Meaning of Research – Characteristics and types of research – Steps of research – Methods of research – Ethics in research – Selection of research topic/problem – Literature collection using primary and secondary sources – Basic elements of experimental work – Analysis of the experimental results and data – Reporting of the results in the form of a research article – Preparation of the scientific research paper for publication in journals and for presentation in scientific seminars, conferences, symposia and workshops . The concept of plagiarism check – The basic characteristics, principles, format and the techniques to be adopted in the preparation or writing of Dissertation and Thesis.	15Hrs
2.	**Basic Computer Concepts –**	15Hrs

	Introduction of Computers: History, Generations and Types of Computers. Hardware: Input Devices, Output Devices, External Memory Storage, CPU. Software: System Software, Application Software Introduction to Word Processing: creating, editing and saving documents, formatting features of word processing, working with tables, graphs and Excel sheet, Presentation basics, creating, saving and displaying	
3	**Chromatography:** Introduction, Definitions, Classifications in Chromatography Adsorption column Chromatography: Types of columns, Experimental requirements, Development of column, Factors affecting column efficiency, Applications and experiments, Separation of (1) Methylene Blue and malachite green (2) Metal ions and (3) Chlorophylls and carotenoids Paper Chromatography: Theory, principles and techniques, development of chromatogram (ascending and descending), 2-Dimensional and Multi dimensional Paper Chromatography, Measurement of R_f values, Applications and Experiments, Separations of (1) Amino acids,(2) Cations and(3) Complexes. Thin Layer Chromatography : Preparation and development of plates, Advantages of TLC, Applications and Experiments, Separation of (1) Ink pigments (2) Dice and (3) Amino acids. High performance Thin Layer Chromatography (HPTLC) – Features and Applications Gas Chromatography: Principles and Theory – Instrumentation, Columns and Detectors, Types of Chromatograms, Analysis of Elution peaks, Applications and Qualitative and Quantitative Analysis. High Performance Liquid Chromatography(HPLC): Introduction, Characteristic feature of HPLC, Comparision of Super Critical fluid, Fluid Chromatography with HPLC and GLC, Principle of HPLC,	15 Hrs

	Instrumentation, Components, Types of Detectors, Reverse phase HPLC and Applications in Organic Chemistry	
4	**Treatment of experimental data:** Errors in Chemical Analysis, precision and accuracy, Methods of Expression of Accuracy, Methods for expression of Precision, the Average Deviation, the Standard Deviation, the Variance, The Relative Standard Deviation, Probable Deviation, Confidence Limit, Classification of Errors, The Determinate and Indeterminate errors, The Normal Law of Distribution of Intermediate Errors, Statistical Tests of Experimental Data, the F-test, the t-test and the Q-test, the Method of Least Squares, Significant figures	15 Hrs

Text Books and References :	
1	Thesis and Assignment Writing by Anderson
2.	Research Methodology and Statistical Analysis by Renu Gambhir
2	Introduction to Computers by Peter Norton
3	Alexis Leon & Mathew Leon: Introduction to Computers with MS-OFFICE-2000, TMH, -2001.
4	Computers in Chemistry by K V Raman
5	Chromatography by B K Sharma
6	An Introduction to Chromatography by H Kaur
7	Quantitative Inorganic Analysis by A I Vogel
8	Fundamentals of Analytical Chemistry by Douglas A Skoog, Donald M West, F. James Holler

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Ph.D in Chemistry
(Syllabus of Paper -2)

Course Code **PHCH102CCT**
Course Title **Advanced Instrumentation**

Scheme of Instruction
Total Duration : **60Hrs**
Periods /Week : **4**
Credits : **4**
Instruction Mode : Lecture

Scheme of Examination
Maximum Score : **100**
Internal Evaluation : **30**
End Semester : **70**
Exam Duration : **3 Hrs**

Course Objectives: The main purpose of this course is to enhance student's Research knowledge on the advanced aspects of various instrumental spectroscopic techniques such as IR, Raman, NMR, ESR and Mass spectroscopy.

Course Outcomes:

Understanding of various instrumental spectroscopic techniques and their applications in the synthesis and analysis of various organic compounds.

Unit	Course Content	Instruction Hours
1.	**Infrared and Raman Spectroscopy** – Theory of Infrared Absorption and Raman Spectroscopy, Sample handling instrumentation (Basic Components) qualitative and quantitative applications. The Vibration-Rotation Spectrum of Carbon Monoxide; Breakdown of the Born-Oppenheimer Approximation; The Interaction of Rotations and Vibrations; The Vibrations of Polyatomic Molecules; The influence of Rotation on the spectra of polyatomic molecules; Analysis by Infrared techniques; Techniques and instrumentation; Vibrational Raman Spectra; Polarisation of light and the Raman effect; Structure determination from Raman and Infrared Spectroscopy; Techniques	15Hrs

	and Instrumentation.	
2.	**NMR and ESR Spectroscopy** **(A) NMR:** Theory of Nuclear Magnetic Resonance Spectroscopy; Quantum description of NMR; Classical description of NMR; Types of NMR spectra; Environmental effect of NMR spectra; the chemical shift; the block diagram of NMR spectrometer; Applications of Proton NMR in qualitative and quantitative analysis in general. **(B) ESR:** Comparison between NMR and ESR; Types of substances with unpaired electrons; Theory of ESR; Instrumentation; Presentation of the ESR spectrum; hyperfine spitting; determination of 'g' value; deviation of the 'g' value; line width; applications of ESR spectroscopy; ENDOR, ELDOR	15Hrs
3	**^{13}C and 2D NMR Spectroscopy** **(A) ^{13}C NMR Spectroscopy:** CW and PFT techniques – Types of CMR spectra – undecoupled – proton decoupled – off – resonance decoupled (SFORD) – Selectivity decoupled and gated decoupled spectra – ^{13}C chemical shifts – Factors affecting the chemical shifts – Homonuclear (^{13}C - ^{13}CJ) and heteronuclear (^{13}C – ^{1}H, ^{13}C-^{2}HJ) couplings. **(B) 2D NMR Spectroscopy:** Introduction; classification of 2D experiments – 2D-J-resolved spectroscopy – HOMO and HETERO – 2D – J – resolved spectra; Correlation Spectroscopy (COSY) – HOMO – COSY, HETERO – COSY, 2D – INADEQUATE and NOESY.	15 Hrs
4	**(A) Mass Spectrometry** Basic principles – instrumentation – ion production – ion analysis – magnetic sector instruments – quadrapole mass spectrometers – time of flight mass spectrometers; ion-cyclotron resonance spectrometers - mass spectrum – molecular ion – types of ions in mass spectra; effect of isotopes on mass spectra; determination of molecular formula;	15 Hrs

	McLafferty rearrangement; meta stable ions; nitrogen rule; general fragmentation modes; mass spectra of hydrocarbons; alkanes (Dodecane 3-3-dimethyl heptanes); cycloalkanes (n-propyl cyclo hexane); alkene (β – Myrcene); alkyne (1-butyne); aromatic hydrocarbons (ethyl benzene and n-butyl benzene) and alcohols (1-pentanol, 2-pentanol, 2-methyl-2-butanol). **(B) Photoelectronic Spectroscopy and X-Ray Crystallography** Introduction, Principle, Instrumentation theory, Application and Comparison with other methods. Auger Electron spectroscopy and Electron spectroscopy for Chemical Analysis- Principle and applications. Experimental techniques- Resolution and Sensitivity of Photo Electron Spectrometer using X-rays, Spectrometer for liquid samples, XRD as Instrumental technique in Chemical Analysis Basic principles. Instrumentation, outlines of procedures and application of X-ray Frutescence.	

Text Books and References:

1	Principles of instrumental analysis by D. A. Skoog
2	Fundamentals of molecular spectroscopy by C. N. Banwell
3	Spectrometric identification of organic compounds by Silverstein
4	Instrumental methods of analysis by Willard and Merritt and Dean
5	Spectroscopy by Chatwal and Anand
6	Organic Spectroscopy by William Kemp
7	IR and Raman Spectra by Nakamoto
8	Molecular structure and spectroscopy by G. Aruldhas
9	Spectroscopic methods in Organic Chemistry by Dudley H. Williams and Ian Fleming

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(Syllabus of Paper –III Ph.D in Chemistry)

Course Code: PHCH101DST
Course Title **Synthesis and Reactivity of Natural Products**

Scheme of Instruction
Total Duration : **60Hrs**
Periods /Week : **4**
Credits : **4**
Instruction Mode : Lecture

Scheme of Examination
Maximum Score : **100**
Internal Evaluation : **30**
End Semester : **70**
Exam Duration : **3 Hrs**

Course Objectives: This paper deals with the study of synthesis and reactivity of natural products. This paper includes 4 units which are i) biosynthesis of natural products, ii) non-aromatic heterocyclic's and aromaticity, iii) synthesis, reactivity, aromatic character and importance of heterocyclic compounds and iv) heterocyclic compounds with more than two hetero atoms.

Course Outcomes: After through study of this paper, students may be able to understand the various methods of biosynthesis of natural products, concept of aromaticity and also gain the knowledge of synthesis and physicochemical properties and importance of heterocyclic compounds containing one or more hetero atoms.

Unit	Course Content	Instruction Hours
1.	**Biosynthesis of Natural Products** Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of biosynthetic precursors, Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by	15Hrs

	chemical degradation and spectral methods. Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway : Biosynthesis of terpenes – mono, sesqui, di, tri (β-amyrin) and carotenoids, steroids – cholesterol	
2.	**Nonaromatic Heterocyclics & Aromaticity** Different types of strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanesandthietanes Aromaticity: Introduction, Aromatic and anti aromatic compounds. Criteria for aromaticity. Huckel's 4n+2 π electron rule for benzene and non benzenoid aromatic compounds. E.g. Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.	15Hrs
3	**Synthesis, Reactivity, Aromatic character and Importance of Heterocyclic Compounds** Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole. OC (CB1) 19:	15 Hrs
4	**Heterocyclic compounds with more than two Hetero Atoms** Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3- triazoies,1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1 ,3,4-oxadiazole, 1,2,5- oxadiazole, 1,2,3-thiadiazoles, 1,3,4- thiadiazoles, 1,2,5- thiadiazoles, 1,2,3-triazine, 1,2,4- triazine, 1,3,5- triazine, tetrazines. Synthesis and importance of purines and pteridines. Syntheis of Caffeine, theobromine and theophylline.	15 Hrs

Text Books and References:

1	I. L. Finar: Organic Chemistry (Vol. I & II), E. L. B. S.	
2	R. T. Morrison & R. N. Boyd: Organic Chemistry, Pearson	

	Education.	
3	Arun Bahl and B. S. Bahl : Advanced Organic Chemistry, S. Chand	
4	Peter Sykes: A Guide Book to Mechanism in Organic Chemistry, Orient Longman.	

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(Syllabus of Paper –IV Ph.D in Chemistry)

Ph.D., (Course Work)

Paper-IV: Research and Publication Ethics

Paper Code:	PHCC104CCT	Semester Exam:	50 Marks
Instruction:	2 h / week	Duration:	30 hours
Credits:	2	Internal Assessment:	15 Marks
		End Semester Exam:	35 Marks

Module	Topic
	THEORY
RPE 01: Philosophy and Ethics (3hrs)	
1.1	Introduction to philosophy: definition, nature and scope, concept, branches
1.2	Ethics: definition, moral philosophy, nature of moral judgements and reactions
RPE 02: Scientific Conduct (5hrs.)	
2.1	Ethics with respect to science and research
2.2	Intellectual honesty and research integrity
2.3	Scientific misconducts: Falsification. Fabrication. and Plagiarism (FFP)
2.4	Redundant publications: duplicate and overlapping publications, salami slicing
2.5	Selective reporting and misrepresentation of data
RPE 03: Publication Ethics (7 hrs.)	
3.1	Publication ethics: definition, introduction and importance
3.2	Best practices/standards setting initiatives and guidelines: COPE, WAME, etc.
3.3	Conflicts of interest
3.4	Publication misconduct: definition, concept, problems that lead to unethical behaviour and vice versa, types
3.5	Violation of publication ethics, authorship and contributor ship
3.6	Identification of publication misconduct, complaints and appeals

3.7	Predatory publishers and journals
PRACTICE	
RPE-04: Open Access Publishing (04 hrs)	
4.1	Open Access Publications and initiatives
4.2	SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies
4.3	Software tool to identify predatory publications developed by SPPU
4.4	Journal finder /journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggested, etc.
RPE 05: Publication Misconduct:	
	A. Group Discussions (2 hrs.)
5.1	Subject specific ethical issues, FFP, authorship
5.2	Conflicts of interest
5.3	Complaints and appeals: examples and fraud from India and abroad
	B. Software tools (2 hrs.)
5.4	Use of plagiarism software like Turnitin, Urkund and other open source software tools
RPE 06: Databases And Research Metrics	
	A. Databases (4 hrs.)
6.1	Indexing databases
6.2	Citation databases: Web of Science, Scopus, etc.
	B. Research Metrics (3 hrs.)
6.3	Impact Factor of journal as per Journal Citation Report, SNIP, SJR, PP, Cite Score
6.4	Metrics: h-index, g index, il0 index, Altmetrics
	Text Books and References:
1	The Ethics in Science -an introduction, David B. Resnil, Routledge, New York 1998
2	Best Practice Guidelines Ethics: A Publishers Perspective, 2nd edition Wiley 2014
3	Levels of Misconduct and Suggested Advice on Actinon to be taken Report from the CSIR Institute of Genomics and Integrative Biology (IGIB), based on material collected from IISER Pune, Oxford University UK and the US Office of Research Integrity
4	Ethicsd in Science Education, Research and Governance, Eds. K. Muralidhar, A. Ghosh, K. Singhvi: Indian National Science Academy, New Delhi, India 2019
5	Bird, A. (2006) Philosophy of Science . Routledge
6	Predatory publishers are competing open access. Nature 489 (7415) 179.