RANI DURGAVATI UNIVERSITY, JABALPUR

Syllabus for Ph.D. Course work in Chemistry

(Under revised Ph.D. Ordinance no.16)
Effective from the Session 2018-19 onward

Course Structure

Course No.	Title of the paper	Credit	Marks
I	Research methodology	4	100
II	Review of published research in the relevant field	3	100
III	Computer application	3	100
IV	Advanced method in chemistry	3	100
VI	Comprehensive viva-voce (Virtual Credit)	3	100
Total	Credits	16	500

A candidate has to obtained 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. program.

I: Research Methodology

Maximum Marks: 100
Minimum Passing Marks: 50
Credits: 4

Unit-I: Research Methods

Problem selection –Literature survey – Familiarity with ideas and concepts of investigation – acquiring technical skills – drawing inferences from data – qualitative and quantitative analysis – accessing the problems – result and conclusions – presenting a scientific seminar – publication of research paper – art of writing of thesis.

Unit-II: Errors Analysis Limiting Errors, Types of errors-

Gross, systematic and random – central value statistical treatments of data – rejection of data – method of least squares – variance and standard deviation – of combination components – uncertainly analysis and treatment of single sample data – linear regression – polynomial regression.

Unit-III:

Sources of data collection: Primary and Secondary.

Methods and Techniques: Survey, case study, Probability and Sampling.

Mean, Standard Deviation, Coefficient of Variation.

Correlation, chi-squared test. Analysis, Q test, Interpretation and Report writing.

Unit-IV: Instrumental techniques

Basic principles and applications of instrumental techniques: Cyclic voltammetry, Gas chromatography, HPLC, IR, UV-Vis., ESR, $^{1}H/C^{13}$-NMR, Mössbauer, TG/DTA/DSC, SEM, TEM, and XRD.

Unit-V: ***Group theory and vibrational Spectroscopy-***

Application of Group theory to arrive at molecular orbital diagrams and molecular vibrations of AB_3, AB_4, AB_5 and AB_6 type molecules. Use of group theory in predicting IR and Raman active modes in molecules of C_{2v} and $C_{3v\ point}$ groups.

Reading materials suggested:

Students are expected to consults standard books, monographs and research journals, for the proposed courses.

II: Review Article

Maximum Marks: 100
Minimum Passing Marks: 50
Credits: 3

Each student shall submit three hard bound copies of a review article separately based on published works in the relevant field of the following subject based on at least 50 relevant up-to-date references for evaluation:

(1) Inorganic Chemistry
(2) Organic Chemistry
(3) Physical Chemistry
(4) Analytical Chemistry

III: Computer Application

Maximum Marks: 100
Minimum Passing Marks: 50
Credits: 3

Unit I

Introduction to Computers and Computing. Basic structure and Components of a computer. Evolution of computational machines, Memory devices. Secondary storage Computer languages. Number systems and some related numerical problems. Operating systems with DOS as an example Introduction to UNIX and WINDOWS. Principles of programming, Algorithms and flow-charts.

Unit II

Use of Computer programmes: Operation of PC. Data Processing. Running of standard Programs and Packages such as MS WORD, MS EXCEL-special emphasis on calculations and chart formations. X-Y plot. Simpson's Numerical Integration method. Programmes with data from physical and inorganic experiments.

Application of Internet for Chemistry with search engines, various types of files like PDF, JPG, RTF and Bitmap. Scanning, OMR, Web camera.

Unit III

Computer Programming in FORTRAN/C/BASIC. (the language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C the features may be replaced appropriately). Elements of the computer language. Constants and variables. Operations and symbols Expressions. Arithmetic assignment statement. Input and output Format statement. Termination statements. Branching statements as IF or GO TO statement. LOGICAL variables. Double precession variables. Subscripted variables.

Unit IV

Internet. Application of Internet for Chemistry with search engines, various types of files like PDF, JPG, RTF and Bitmap. Scanning, OMR, Web camera.

Unit V

Origin of Computational Software Models**:** Quantum Mechanics and its general applications in chemistry, Schrodinger's time dependant and time independent equations with derivations. Historical background of DFT approach, Thomas Fermi model and Kohn Sham Derivations.

Reading materials suggested:

Students are expected to consults standard books, monographs and research journals, for the proposed courses.

IV: Advanced method in chemistry

Maximum Marks: 100
Minimum Passing Marks: 50
Credit: 3

Unit-I:

(a) Group theory and vibrational Spectroscopy: Application of Group theory to arrive at molecular orbital diagrams and molecular vibrations of AB_3, AB_4, AB_5 and AB_6 type molecules. Use of group theory in predicting IR and Raman active modes in molecules of $C_{2v}$and C_{3v} point groups.

(b) *MO treatment of bonding:* Molecular orbital treatment of bonding in Cu_2O, $C_nO_n^{2-}$, BF_3, $Fe(C_5H_5)_2$, $Cr(C_6H_6)_2$, boranes.

Unit-II:

Mössbauer Spectroscopy. Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate spin, (2) Sn^{+2} and Sn^{+4} compounds –nature of M-L bond, coordination number, structure and (3) detection of oxidation state.

Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD). Concept of ORD and CD. Structural elucidation of coordination compounds.

Unit-III

(a) *Microwaves in organic synthesis.* Nonthermal effects of microwaves in organic synthesis. Origin of microwave effects. Specific microwave effects. Effect of the medium. Effects of reaction mechanisms. Selectivity in microwave assisted reactions. Advantages and limitations of microwave heating in organic synthesis.

(b)*The Disconnection Approach*. Basic principles, synthons, functional group interconversions. Order of events in organic synthesis. One group C-X disconnections and two group C-X disconnections.

Unit-IV:

Instrumental techniques: Basic principles and applications of instrumental techniques: Cyclic voltammetry, Gas chromatography, HPLC, IR, UV-Vis., ESR, $^{1}H/C^{13}$-NMR, Mössbauer, TG/DTA/DSC, SEM, TEM, and XRD.

Conjoint Spectroscopy Problems: Application of UV, IR, Raman, NMR, and Mass spectrometry for elucidation of structure of organic and inorganic compounds.

Unit-V:

(a) *Homogeneous catalysis by transition metal complexes*: Hydrogenation of olefins, asymmetric hydrogenation, hydrosilation and hydroboration reactions. Hydroformylation of unsaturated hydrocarbons. Zeigler-Natta polymerization-mechanism.

(b) *Medicinal Inorganic Chemistry*: Potentiality of metal complexes as antihypertensive and anticancer agents. Metal complexes as Insulin adjuvant-probable mechanism. Bioinorganic chemistry of Pt-anticancer drugs; how they work? Chelation therapy in Alzheimer disease.

Reading materials suggested:

Students are expected to consults standard books, monographs and research journals, for the proposed courses.

V: Comprehensive viva-voce

Maximum Marks: 100
Minimum Passing Marks: 50
Credit: 3