

# SYLLABUS FOR Ph.D. COURSE WORK CHEMISTRY (ONE SEMESTERS COURSE)

## Choice Based Credit System (CBCS) Syllabus: Effective from July 2016

The Ph.D. Course work Chemistry shall have one semester course. The numbers of papers in this course, along with their credits are given below. It is necessary to secure minimum 50% passing marks in all the papers separately. The Course is governed by the **University Ordinance No. 16**.

### I: Research Methodology

**Maximum Marks: 100**  
**Minimum Passing Marks: 50**

Credits: 5

#### Unit-I:

(a) *Group theory and vibrational Spectroscopy*: Application of Group theory to arrive at molecular orbital diagrams and molecular vibrations of AB<sub>3</sub>, AB<sub>4</sub> and AB<sub>6</sub> type molecules. Use of group theory in predicting IR and Raman active modes in molecules of C<sub>2v</sub>, C<sub>3v</sub> and D<sub>∞h</sub> point groups.

(b) *MO treatment of bonding*: Molecular orbital treatment of bonding in hydrazoic acid/hydrazide ion, Cu<sub>2</sub>O, C<sub>n</sub>O<sub>n</sub><sup>2-</sup>, Fe(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>, Cr(C<sub>6</sub>H<sub>6</sub>)<sub>2</sub>, borane and metal clusters.

#### Unit-II:

(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.

#### 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, <sup>1</sup>H/<sup>13</sup>C-NMR, Mössbauer, TG/DTA/DSC, SEM, TEM, and XRD.

#### Unit-V

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

#### Reading materials suggested:

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

## II: Computer Application

**Maximum Marks: 50**  
**Minimum Passing Marks: 25**

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

*Programming in Chemistry.* Developing of small computer codes using any one of the languages FORTRAN/C/BASIC involving simple formulae in Chemistry, such as Van der Waals equation. Chemical kinetics (determination of Rate constant) Radioactive decay (Half Life and Average Life). Determination Normality, Molarity and Molality of solutions. Evaluation Electronegativity of atom and Lattice Energy from experimental determination of molecular weight and percentage of element organic compounds using data from experimental metal representation of molecules in terms of elementary structural features such as bond lengths, bond angles.

### Unit III

*Use of Computer programmes and Internet.* 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 IV

**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.

### Unit V

**Current Use of Software Packages in Chemical Research:** Gaussian and GaussView, Hartree-Fock Theory and Basis Sets, Semi empirical Methods, Electron Correlations, Density Functional Theory, Combined QM/MM Methods, Why and How to Combine QM and MM, Solvation and Solvent Effects, Polarization, Reaction profiles in solution, Protein-Ligand Interactions, Modeling Enzymatic Reactions

**Books Recommended**

1. Quantum Chemistry, 6<sup>th</sup> ed., Ira N. Levine, Pearson Education, Inc., New Delhi, 2012
2. Molecular Quantum Mechanics, 4<sup>th</sup> ed., P. W. Atkins, R. S. Friedman, Oxford University Press 2005
3. Essentials of Computational Chemistry, 2<sup>nd</sup> ed., C. J. Cramer, Wiley, 2005
4. Introduction to computational Chemistry, 2<sup>nd</sup> ed., F. Jensen, Wiley, 2007
5. Computational Chemistry, D. Young, Wiley 2001
6. Fundamentals of Computer: V. Rajaraman, Prentice Hall.
7. Computers in Chemistry: K.V. Raman, Tata Mc Graw Hill).
8. Computer Programming in FORTRAN IV-V Rajaraman, Prentice Hall.
9. Computers and Common Sense, R. Hunt and J. Shelley, Prentice Hall.
10. Computational Chemistry, A.C. Norris.
11. Microcomputer Quantum Mechanics, J.P. Killngbeck, Adam Hilger.
12. An Introduction to Digital Computer Design, V. Rajaraman and T. Radhakrishnan, Prentice Hall.

### III: Review of Published Research in the relevant field

**Maximum Marks: 50**  
**Minimum Passing Marks: 25**

Credits: 3

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

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

### IV: Comprehensive Viva

**Maximum Marks: 50**  
**Minimum Passing Marks: 25**

Credits: 4