বিদ্যাসাগর বিশ্ববিদ্যালয়

Vidyasagar University

Department of Chemistry

Syllabus: Ph.D. Coursework

Course Structure of the Ph.D. Course work in Chemistry

<table>
<tr><th colspan="2">Course</th><th>Subject</th><th>Full Marks</th><th>Credit Hours</th></tr>
<tr><td>Compulsory Unit</td><td>Course I</td><td>Research Methodology</td><td>50</td><td>16</td></tr>
<tr><td rowspan="3">Elective Units</td><td colspan="4">Choose any two (02) of the following courses as Course II and III</td></tr>
<tr><td>Course II</td><td rowspan="2">1. Frontiers in Organic Chemistry
2. Advanced Photophysics and Computational Chemistry
3. Advanced Inorganic and Bio-inorganic Chemistry
4. Biophysical Chemistry and Surface Chemistry
5. Biological Organic Chemistry and application of advanced techniques to study modes of interaction</td><td>50</td><td>16</td></tr>
<tr><td>Course III</td><td>50</td><td>16</td></tr>
<tr><td>Compulsory Unit</td><td>Course IV</td><td>Review of Research Work
[A Literature Review or data generated on the related research topic be submitted by each scholar duly signed and recommended by the Supervisor]</td><td>50</td><td>-</td></tr>
</table>

Compulsory Unit

Course I

(Marks 50)

Research Methodology:

Definition of problem: Necessity of defining problem, Technique involved in defining a problem. Surveying the available literature.

Techniques involved in solving the problem: Different methods used to solve a problem.

Research Design: Subject of study; Place of study; Reason of such study; Type of data required; Method of data collection; Periods of study; Style of data presentation.

Developing a research plan: Research objective; Information required for solving the problem; Each major concept should be defined in operational terms; An overall description of the approach should be given and assumption if considered should be clearly mentioned in research plan; The details of techniques to be adopted.

Methods of data collection*:* Experimental methods.

Analysis of data: Various measures of relationship often used in research studies, Correlation coefficients.

Elective Units

Course II

(Marks 50)

and

Course III

(Marks 50)

Choose any two (02) of the following courses

as Course II and Course III

1: Frontiers in Organic Chemistry

1. Green Chemistry: Principles of Green Chemistry, Examples, Renewables for Sustainability, Green Synthesis, Plant secondary metabolites, Terpenoids: Biogenesis, Biosynthesis, Triterpenoids as Renewable Nano-entities
2. Computational Chemistry: Classical mechanical approach for the determination of structures of organic compounds and its application in synthesis and molecular recognition
3. Self-assembling systems: vesicles, fibers, spheres, tubules, gels; study of their morphologies and properties; applications in, drug delivery, thermochromic materials
4. Seminar lectures by students on a recently published paper in organic chemistry

Suggested Reading:

1. *Molecular Gels: Materials with Self-Assembled Fibrillar Networks*. Weiss, Richard G., Terech, Pierre (Eds.), 2006, Springer
2. *Green Chemistry: Theory and Practice*. Paul T. Anastas, John Charles Warner. Oxford University Press, 1998
3. *Green Chemistry: Principles and Practice*, P. Anastas, N. Eghbali, *Chem. Soc. Rev.* 2010, 301-312.
4. *Molecular Mechanics*, N. L. Allinger, Theoretical and Computational Models for Organic ChemistryFormosinho, S.J., Csizmadia, Imre G., Arnaut, Luìs G. (Eds.) pp 125-135; 1991, Springer
5. B.G. Bag, R. Majumdar, Self–assembly of renewable nano–sized triterpenoids, *Chem. Rec.* 2017, *17*, 1, 1-34.
6. B. G. Bag, A. C. Barai, S. N. Hasan, S. K. Panja, S. Ghorai, *S. Patra, Pure Appl. Chem* S. Patra., 2020, *92*, 567-577.

2: Advanced Photophysics and Computational Chemistry

Shapes of absorption band and Franck-Condon principle, Emission spectra, Environmental effect on absorption and emission spectra, Excited state dipole moment, Excited state acidity constant, Time resolved emission. Bimolecular collision and the mechanism of fluorescence quenching, Kinetics of collisional quenching: Stern-Volmer equation, concentration dependence of quenching, excimer & exciplex.

Radiative energy transfer: Forster resonant energy transfer (FRET), photoinduced electron transfer.

Computational Chemistry:

Semi-empirical method: MNDO, AM1, PM3

Ab-initio implementation of Hartree-Fock MO theory, Basis sets, key technical and practical points of HF theory. General performance overview of ab-initio HF theory.

Density Function theory: Theoretical motivation, philosophy, Kohn-Sham self-consistent field methodology. Advantages and disadvantages of DFT compare to MO theory. General performance overview of DFT, case study.

References:

1. Principles of fluorescence spectroscopy by J. R. Lakowicz; CRC Press
2. Photophysics of Aromatic Molecules by J. B. Birks; Wiley Interscience
3. Essential of computational chemistry by Christopher J. Cramer; Wiley

3. Advanced Inorganic and Bio-inorganic Chemistry

Application of advanced techniques to study micro and macromolecular interaction

Interaction of complexes with DNA, RNA and Serum proteins (Bovine serum albumin (BSA) and Human serum albumin (HSA), Human haemoglobin and myoglobin etc.) monitored by (a) UV-Vis spectroscopy (b) UV-thermal melting (c) Fluorescence spectroscopy (d) Cyclic voltammetry (e) Circular dichroism spectroscopy (CD) and (f) Isothermal titration calorimetry (ITC).

Interaction between nanoparticle and Serum proteins (Bovine serum albumin (BSA) and Human serum albumin (HSA), Human haemoglobin and myoglobin etc.) monitored by (a) UV-Vis spectroscopy;(b) UV-thermal melting (c) Fluorescence spectroscopy and 3D fluorescence spectroscopy; (d) DLS and Zeta potential measurement study; (e)IR-Spectroscopy;(f) Circular dichroism spectroscopy (CD) and (f) Isothermal titration calorimetry (ITC).

Advanced OrganometallicChemistry

Representative organometallic reactions with a special reference to the reaction mechanism.

Stereochemical non-rigidity and fluxional behaviour of organometallic compounds.

Metallocene: η5 - Cyclopentadienyl metal complexes, η6 -Arene metal complexes,

Catalysis by organometallic compounds: Wilkinson's catalyst, Tolman's catalytic loops; Synthesis gas, Water gas shift reaction, Synthesis of methanol, Hydroformylation (oxo process), Hydrogenation of unsaturated compounds, Monsanto acetic acid process, Wacker process, Synthetic gasoline, Fischer-Tropsch process and Mobil process; Polymerisation, Oligomerisation and metathesis reactions of alkenes and alkynes; Ziegler-Natta catalysis.

Magnetic Properties of Materials

Ferromagnetism, Ferrimagnetism, Antiferromagnetism, Magnetic Susceptibility *vs.* Temperature, Metamagnet, Superparamagnet, Paramagnetism in Metal Complexes, Hysteresis Curves, Antiferromagnetism in Metal Oxides, Super-exchange, Magnetic

Ordering in Rock Salt Oxides, Magnetic interaction in polynuclear metal complexes, MOFs as magnetic materials.

Suggested Readings:

1. In Drug-DNA Interaction Protocols, Second Edition, Yang Liu, W. David Wilson (auth.), Keith R. Fox (eds.) Springer New York.
2. Circular Dichroism and the Conformational Analysis of Biomolecules Jen Tsi Yang (auth.), Gerald D. Fasman (eds.) Springer US.
3. Analytical Applications of Circular Dichroism, Volume 14 1st Edition, N. Purdie H.G. Brittain, Elsevier Science.
4. B. D. Gupta and A. J. Elias 2010, Basic Organometallic Chemistry: Concepts, Syntheses and Applications, Universities Press, Hyderabad.
5. J. P. Collman, L.S. Hegedus, J.R. Norton and Richard G. Finke, 1987, Principles and Applications of Organotransition Metal Chemistry, 1st Edtion, University Science Books, Mill Valley, California.
6. Gerard Jaouen (Ed.), 2005, Bioorganometallics, Wiley-VCH.
7. Elements in Magnetochemistr, R. L. Dutta and A. Shyamal, Affiliated East-West Press.
8. Solid State Physics, S. O. Pillai, New Age International Publishers.

4: Biophysical Chemistry and Surface Chemistry

Thermodynamics in Biochemistry (Fundamentals and Applications); Biopolymers (Proteins, Enzymes, DNA, Carbohydrates); Biomembranes (Structure and Function); Active transport and passive transport, Multiple equilibria, Specific examples of multiple equilibria, Transport processes; General features of transport processes; Optical systems for the study of transport processes.Self-organizing systems: Their interactions, Physico-chemical Properties, Different Characterization techniques, Applications. Preparation, Characterization and Application of nanoparticles Surface and Biophysical Techniques: Calorimetry, CD, SEM, TEM, EDAX, DLS, Gel Electrophoresis, Radioactivity, XPS.

Suggested Readings:

1. Thermodynamics and an Introduction to Thermodynamics, H. B. Callen
2. Principles of Physical Biochemistry, K. E. van Holde, C. Johnson, P. S. Ho
3. Physics and Chemistry of Interfaces, Hans-Jürgen Butt, Karlheinz Graf, Michael Kappl
4. Physical Chemistry of Surfaces, Arthur W. Adamson, Alice P. Gast
5. Physical Chemistry of Macromolecules, C. Tanford
6. Polymer Chemistry, P. J. Flory
7. Nanocrystals: Synthesis, Properties and Applications, C.N.R. Rao, P. John Thomas, G. U. Kulkarni

5: Biological Organic Chemistry and application of advanced Techniques to study modes of interaction

Nucleic Acids: DNA; Structural features of various forms of DNA; RNA; Various types of RNA and their structural properties and function.

Alkaloid-Nucleic Acid Interactions and its Implications for Drug Design: Isoquinoline alkaloids and their medicinal properties; Binding of small molecules to nucleic acids; Interaction of berberine, palmatine, coralyne, jatrorrhizine and sanguinarine with various forms of natural and synthetic DNAs and RNAs; Binding of derivatives of the alkaloids with nucleic acids; The mode, mechanism and thermodynamics of the alkaloid-nucleic acid binding interaction monitored by (a) UV-Vis spectroscopy;(b)UV-thermal melting (c) Fluorescence spectroscopy; (d) Cyclic voltammetry ; (e) Circular dichroism spectroscopy(CD) and (f) Isothermal titration calorimetry (ITC).

Suggested Readings:

1. In Drug-DNA Interaction Protocols, Second Edition, Yang Liu, W. David Wilson (auth.), Keith R. Fox (eds.) Springer New York
2. Circular Dichroism and the Conformational Analysis of Biomolecules Jen Tsi Yang (auth.), Gerald D. Fasman (eds.) Springer US
3. Analytical Applications of Circular Dichroism, Volume 14 1st Edition, N. Purdie H.G. Brittain, Elsevier Science
4. Biophysical, Chemical, and Functional Probes of RNA Structure, Interactions and Folding: Part A Andrew L. Feig, in Methods in Enzymology. Elsevier
5. Data Processing Handbook for Complex Biological Data Gauri Misra, Academic Press
6. Nucleic acids structure and recognition, by Stephen Neidle, Oxford University Press, 2002.
7. Principles of Nucleic Acid Structure by Stephen Neidle, 1st Edition, Academic Press.

Compulsory Unit

Course IV

(Marks 50)

Review of Research Work

Assignment to be submitted

[A Literature Review or data generated on the related research topic be submitted by each scholar duly signed and recommended by the Supervisor]