

2106

DEPARTMENT OF CHEMISTRY
PATNA UNIVERSITY
Syllabus for Course-Work

Ph.D in Chemistry

Paper -II

In this paper, there are two groups. The group A is compulsory and includes the principles of Spectroscopy which improves the knowledge in the spectral studies of compounds related with the research work through their special data. This will help the students in the analysis of the compounds.

The group B is optional containing three sections and the students have to opt any one section from this group

Group-A (Compulsory)

- 1. General spectroscopy:** General principles, factors influencing vibrational frequencies, selection rules, Analysis of infra-red technique, Fourier transform, IR-spectroscopies. Introduction of terahertz spectroscopy, Application of IR and terahertz spectroscopy, Far IR spectra of inorganic and organic compounds
- 2. Electronic spectroscopy:** Basic principles of electronic absorption spectra of organic and inorganic molecules, Selection rules and their implication, Instrumentation, Analytical applications, qualitative and quantitative analysis
- 3. NMR spectroscopy:** Nuclear magnetic resonance spectroscopy: General principles, sensitivity of the method, CW and FT- NMR instrumentation, Application in chemical analysis (with special reference ^1H , ^{13}C and ^{19}F NMR chemical shift, spin-spin splitting, area of peak, shift reagents, off-resonance decoupling, Nuclear overhauser effect, solid state and gas phase NMR spectra.
- 4. Mass spectroscopy:** Mass spectrometry: Principles, advantages and limitations of mass spectroscopy. Instrumentation, Method of ionization, Metastable fragmentation pattern. Theory of mass spectrometry. structural elucidation of inorganic and organic compounds
- 5. X-ray diffraction and X-ray photoelectron spectroscopy:** Basics principle and applications.
- 6. Electron Paramagnetic Resonance:** Basic principles, Isotropic hyperfine effects, Zeeman energy, anisotropy, hyperfine anisotropy applications.
- 7. Mossbauer spectroscopy:** Fundamentals of Mossbauer spectroscopy and applications.

Suggested books

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1. C.N. Banwell fundamentals of molecular spectroscopy (4th edition) Tata mcGraw Hill, New Delhi, 1994
2. R.M.Silverstein, G.C. Bassler. C.Morril, spectrometric identification of organic compounds (5th edition) John wiley and sons, 1991
3. J.R.Lakowicz, principle of Fluorescence spectroscopy (3rd edition), 2006
4. J.R.Lakowicz, principle of Fluorescence spectroscopy (3rd edition), 2006
5. D.L.Pavia, G.M.Lampman, G.S.Kriz, Introduction of Spectroscopy(3rd edition), Thomson Brooks/Cole, 2000.
6. Fritz Helmet, Mossbauer spectroscopy
7. J.A.Weil, and J.R.Weil, and J.R.Bolton, Electron paramagnetic Resonance: Elementary Theory and Practical Applications.

Section I

Physical Chemistry (optional)

Introduction: Introduction to nano scale and colloidal system, fundamentals of surface and interfacial Chemistry, surface tension and wettability Insoluble monolayers

Adsorption phenomena: Adsorption of surfactants of solid surface. Langmuir adsorption and models describing multilayer adsorption; miscelles and micro emulations.

Immobilization of biomolecules: strategies and applications in nanobiotechnology,

Heterogeneous catalysis: Historical background : Catalysis, Difference between homogeneous and heterogeneous catalysis, Reactive interfaces; Effect of structure on reactivity; Catalytic materials and their preparation; activity and selectivity, Measurement of catalytic properties, Application in raw materials and their conversions, Environmental protection and daily life; Future of catalysis

Suggested books

1. D. Fennell Evans and Hakan Wennerstrom; The colloidal Domain: where physics, Chemistry, Biology and Technology Meet, 1999 John-Wiley and sons, Inc.
2. By K.S.Birdi, Handbook of surface and colloid chemistry 2008 CRC Press.
3. Gabor A. Somorjai, Yimin Li, Introdction to surface chemistry and catalysis 2010 John-Wiley and sons.
4. T.Pradeep, Nano: The Essentials 2007 Tata MaGraw-Hill.
5. Chad A. Mirkin, Christof M. Niemeyer, Nanobiotechnology II: More concepts and Applications 2007 Wiley-vch Verlag Gmbh.

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6. Bowker Michael, *The Basis and Applications of Heterogenous Catalysis* 1998 Oxford University Primer.
Research articles in the journals.

Section II

Inorganic Chemistry (optional)

1. General aspect of bonding in inorganic molecules and coordination complexes; Different theories like valence bond, crystal Field; Molecular orbital and Ligand field theory, Magnetic properties, Ferromagnetic and antiferromagnetic, paramagnetic-diamagnetic substances, and Curies Law. Magnetic exchange interaction; spin state equilibrium; temperature dependent paramagnetism
2. Electronic spectroscopy and IR spectral measurement used for structural elucidation.
3. Application of group theory for structural and spectral studies of complexes molecules
4. X-RD and X-ray analysis of complex molecule for the complex structure frame-work;
5. Techniques involved in micro investigation like antibacterial, antifungal and antitumoral activities.
6. **Metal organic frameworks:** Development of metal organic materials, guest removal and uptake, flexibility, topology and interpenetration; highly connected metal organic framework; organometallic network, acentric and chiral network, application of metal-organic framework in nonlinear optics, selective absorption of gas and vapour, hydrogen, methane; Carbon dioxide storage, Magnetic materials.

Suggested books

1. C.P.Poole and F.J. Owens, *Introduction to Nanotechnology*, Wiley-India 2006.
 2. G.A. Ozin, C. Andre and L.Arsenault, *Nanochemistry : A hemical Approach to nanomaterial*. Royal society of chemistry, 2005
 3. T. Pradeep *NANO: The Essentials* Tata-McGraw Hill's New Delhi 2007
 4. K.J.Kalbunde, *Nanoscale Materials in chemistry* Wiley-interscience 2001.
 5. Bharat Bhushan(Ed.) *Springer Handbook of Nanotechnology* Springer, 2007
- Some recent publication in the reputed general

Section III

Organic chemistry (optional)

1. **Natural products:** Technique of isolation, separation and characterisation by instrumental techniques
2. **Principles of asymmetric synthesis:** Selectivity in synthesis, stereo specific reactions, stereoselective reaction in Enantio selectivity and diastereo selectivity, conditions for

1.1.1.1

2.2.2.2

3.3.3.3

4.4.4.4

5.5.5.5

stereoselectivity, symmetry and transition state criteria, kinetic and thermodynamic control, method for inducing enantio and diastereoselectivity.

3. **Analytical method:** % Enantiomer excess, % enantioselectivity, optical purity, % diastereometric excess and % diastereoselectivity. Techniques for determination of enantioselectivity: specific rotation, chiral ^1H NMR, chiral lanthanide shift reagents and chiral HPLC, GC

4. Methodology of asymmetric synthesis

Classification of asymmetric reactions: (a) substrate controlled (b) Chiral auxiliary controlled. (c) chiral reagent control and (d) Chiral catalyst controlled reactions.

5. Techniques used in organic synthesis:

Purification and enrichment of solvents, drying techniques, Recrystallisation, Chromatography, Interpretation of IR, UV, NMR, Mass spectra of organic molecules.

Suggested Books

1. Nasipuri, D., stereochemistry of Organic Compounds, New Age Publications, 2nd Ed., 1994
2. Eliel, E. Et.al stereochemistry of organic compounds, Wiley-Interscience, 1994.
3. Carruthers, et.al. Modern Methods of Organic synthesis, Cambridge University Press, 4th Ed. 2005
4. Robert E. Gawley, R.E. Gawley, J. Aube, Principles of Asymmetric Synthesis Pergamon Title, Annotated Ed. 2004.
5. Nogradi M.; Stereoselective synthesis: A practical Approach Wiley- VCH 2nd Ed. 1994
6. List B. et. al. Asymmetric organocatalysis Springer 1st Ed. 2010
7. Song C.E.; Cinchona Alkaloids in synthesis and catalysis: Ligands Immobilization and Organocatalysis Wile-vch Verlag Gmbh, 2009

Some recent publications in the reputed journal:

In this course a PG students has to present seminar/presentation or a series of presentations for series representation on a topic(s) chosen by him/her in consultation with his/her Ph.D. Thesis Supervisor/Faculty Advisor. The frequency of seminar presentation will be decided by the course coordinator

Smith
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MP
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OCinglu
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Enemg
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Lucy
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