Approved in 45th BoA Meeting (18-02-22)

Course number : CY-515
Course Name : Advanced Inorganic Spectroscopy
Credit Distribution :*3-0-0-3*
Intended for : PG and PhD level
Prerequisite : Basic understanding of physical chemistry and preliminary knowledge of quantum mechanics, or with instructor's approval.
Mutual Exclusion : None

1. Preamble

Elucidation of chemical and electronic structure of molecules using spectroscopic techniques is one of the most significant aspects of chemistry. Spectroscopy provides conclusive evidence about structure and reactivity. This course enables the students to learn fundamental principles of advanced inorganic spectroscopic techniques that are frequently used in chemistry.

2. Course Modules with quantitative lecture hours

Module 1: Electron Paramagnetic Resonance Spectroscopy (10 hours)

Origin of EPR signals, g-factor, Presentation of the EPR spectrum, Hyperfine splitting: from protons and from Nuclei I > 1/2, Origin of hyperfine interaction, Contributions to the hyperfine interactions in isotropic systems, Anisotropic Effects: Anisotropy in the g value, EPR of triplet states, nuclear quadrupole interaction, line widths, Experimental considerations and application of EPR.

Module 2: Magnetic Circular Dichroism Spectroscopy (6 hours)

Differences with CD, Theoretical Framework: Definition of MCD Terms, Measurement of MCD Spectra, The Interpretation of MCD Spectra, Case Studies; Diamagnetic Systems (A and B terms) and Paramagnetic Systems (C Terms) Magnetic Vibrational Circular Dichroism (MVCD) and X-Ray magnetic Circular Dichroism (XMCD), Application.

Module 3: Nuclear Quadrupole Resonance Spectroscopy (6 hours)

Nuclear quadrupole moment, Energies of nuclear quadrupole transitions, Effect of magnetic field on the spectra, Relationship between electric field gradient and molecular structure, Applications, Interpretations of structural information from NQR spectra.

Module 4: Mössbauer Spectroscopy (7 hours)

The Mössbauer effect, Line width, Recoil energy, Mössbauer active nuclei, Isomer shift, Quadrupole splitting, Magnetic hyperfine interactions, Mossbauer spectroscopy vs. Chemical bond, Structure determination and Analytical applications.

Module 5: **Photoelectron Spectroscopy (6 hours)**

Auger electron spectroscopy, Photoionization process, Spin-orbit Coupling, X-ray Photoelectron spectroscopy, Electron Energy Loss Spectroscopy (EELS).

Module 6: X-ray Absorption and Emission Spectroscopy (7 hours)

Introduction of X-ray absorption spectroscopy (XAS), X-ray emission spectrum (XES), X-ray Absorption spectrum, Theory of X-Ray Absorption Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS), Application.

Laboratory/practical/tutorial Modules:0

3. Text books:

1. **D. N. Sathyanarayana.,** Handbook of Molecular Spectroscopy: From Radio waves to gamma rays, I. K. International Publishing House Pvt. Ltd. 2019.
2. **Russell S. Drago,** Physical Methods in Inorganic Chemistry, Publishers:Van Nostrand Reinhold, 2016.

4. References:

1. **Jack D. Graybeal,** Molecular Spectroscopy, McGraw Hill Education Private Limited, 1988.
2. **G. Aruldhas,** Molecular Structure and Spectroscopy PHI Learning Private Limited, Delhi, 2019.
3. **Editor(s): Jeroen A. Van Bokhoven, Carlo Lamberti,** X- Ray Absorption and X- Ray Emission Spectroscopy: Theory and Applications, John Wiley & Sons, Ltd, 2016.
4. **Editors: Edward I. Solomon, A. B. P. Lever,**Inorganic Electronic Structure and Spectroscopy, Volume I: Methodology and Volume II: Application and Case Studies, John Wiley & Sons, Inc., 2006.
5. **Skoog, West and Holler,** Fundamentals of Analytical Chemistry Publishers: Saunders's College publishing, 2013.
6. **W. Roy Mason,** A Practical Guide to Magnetic Circular Dichroism Spectroscopy, Wiley-Interscience, 2007.

7. Similarity with the existing courses: NA
(Similarity content is declared as per the number of lecture hours on similar topics)

S. No.		Course Code	Similarity Content	Approx. % of Content
1.				

6. Justification of new course proposal if cumulative similarity content is >30%: NA