

NMR spectroscopy (KDIT08)

syllabus

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1. Overview and classification of spectroscopic methods, description of basic physical concepts (macroscopic and microscopic approaches). Electromagnetic waves and their characteristics: quantum energy, relationship between wavelength, wave number, and frequency. The complete electromagnetic spectrum.
2. General laws governing optical spectroscopy: Spectral ranges (radio waves, microwaves, infrared, visible, ultraviolet, X-rays, gamma rays) and their corresponding energies. The design of classical spectrophotometers. Block diagram of an NMR spectrometer.
3. Information obtainable from the spectrum: wavelength, absorbance, and their use for analytical purposes. Basics of qualitative analysis: the application of different wavelength ranges and their information content.
4. Fundamentals of magnetic resonance spectroscopy. Magnetic moment of the atomic nucleus. Measurable atomic nuclei. Theoretical fundamentals of measurement: Larmor precession, Bloch equations, relaxation.
5. Chemical shift, the delta scale. Determining chemical structure using chemical shift. Chemical equivalence. Simple examples.
6. Indirect coupling constant (J). Multiplicity, first-order decay. Use of the coupling constant to determine the configuration and conformation of a molecule. Decoupling. Magnetic equivalence, nomenclature of spin systems.
7. Direct coupling. Solid-state measurements – CP-MAS. Oriented systems (liquid crystals, membranes). Effect appearing in the isotropic phase: Overhauser effect.
8. Spectroscopy of different nuclei. The role of natural isotope abundance: ^1H – ^{31}P , ^1H – ^{19}F spectrum. Dilute nuclei: ^1H – ^2D , ^1H – ^{13}C spectrum from both sides of the nucleus, interpretation of satellite lines. Selective and broadband detachment.
9. Molecular structure and NMR spectrum. Comparison of NMR and IR.
10. Evaluation of one-dimensional NMR spectra I.
11. Evaluation of one-dimensional NMR spectra II.
12. Evaluation of one-dimensional NMR spectra III.
13. Evaluation of one-dimensional NMR spectra IV.
14. Recording of one-dimensional NMR spectra