

Name: Spectroscopy (C-PS.II2-SPECTRO)

Name in Polish:

Name in English: Spectroscopy

**Information on course:**

Course offered by department: *missing department name in English*

Course for department: Faculty of Chemistry

**Default type of course examination report:**

Grading

**Language:**

English

**Course homepage:**

<http://www.umcs.pl/pl/staff-department-of-chromatographic-methods,8641.htm>

**Description:**

Lecture:

Vibrational Spectroscopy. Potential energy curve and (hyper)surface. Equilibrium geometry of a molecule. One-dimensional harmonic oscillator (selection rules, spectrum). Anharmonicity (selection rules). Normal and group vibrations (classification, examples).

Fundamentals of IR spectroscopy – types of vibrational transitions, selection rules, methodology. IR-active/inactive vibrations. Group vibrations of the main groups of organic compounds. Applications of vibrational spectroscopy in the analysis of organic compounds. Hydrogen bonding and its effect on a vibrational spectrum.

NMR spectroscopy. Nuclear spin. Nuclear magnetic moment and its interaction with an external magnetic field. The essence of the nuclear magnetic resonance. Shielding of a nucleus – mechanisms, the magnetic shielding constant, NMR spectrum. Chemical shift, internal standards. Spin-spin coupling and spin-spin coupling constant. Methodology – the effect of a magnetic field strength, integrated curve etc. The <sup>1</sup>H NMR spectroscopy: chemical shifts, the number of signals on the spectrum, the multiplicities of signals. Applications of <sup>1</sup>H NMR spectroscopy in analysis of organic compounds. Hydrogen bonding and its effect on <sup>1</sup>H NMR spectrum, dynamical effects in NMR. <sup>13</sup>C NMR spectroscopy: fundamentals, proton decoupling, chemical shifts, the number of signals on the spectrum, examples of spectra.

Electronic spectroscopy. The electronic transitions of atoms and molecules – selection rules. Methodology. Electronic spectra of simple molecules. Applications of electronic spectroscopy in analysis of organic compounds: chromophores, auxochromes. Examples of electronic spectra of C=C, C=O, OH, NO<sub>2</sub> containing compounds. Luminescence. Quantitative analysis – examples.

Mass spectrometry. Physical fundamentals. The selected techniques of the sample ionization (EI, CI, SIMS, FD, FAB, MALDI etc.). The selected analyzers (magnetic field deflection analyzer, ion trap, quadrupole mass filter, time of flight analyzer). Methodology. Fragmentation process. Mass spectra of the selected groups of compounds. Applications of mass spectrometry (determination of the molecular weight and empirical formula of a compound).

Laboratory:

Fundamentals of spectroscopy: fundamental spectroscopic constants, electromagnetic radiation, basic units characterizing the energy quanta (calculations of the conversion factors), energy forms and their quantization, a spectrum: definition, origin, classification of spectra, transition probabilities, selection rules, bandwidths, background, noise, and integrated intensity

Vibrational Spectroscopy: diatomic molecules: potential energy curve, equilibrium bond length, dissociation limit and energy, polyatomic molecules: internal coordinates, potential energy (hyper)surface, equilibrium geometry, one-dimensional harmonic oscillator: classical and quantum approaches, vibrational spectrum of a molecule within the harmonic approximation (force constant, selection rules), anharmonicity and its effect on the vibrational spectrum (selection rules), polyatomic molecules: vibrational degrees of freedom, normal modes and group vibrations, fundamentals of IR spectroscopy: IR-active and IR-inactive vibrations, types of the vibrational transitions, single and double beam IR spectrometers, CW and FT techniques in vibrational spectroscopy, IR spectrometer (demonstration), recording of the IR spectra of the gas-, liquid-, and solid-phase samples, interpretation of the IR spectra: regions in the vibrational spectrum, group vibrations for various groups of organic compounds (names, notation), correlation tables, hydrogen bonding and its effect on the vibrational spectrum, carbonyl group stretching vibration: the influence of inductive and mesomeric effects, determination of a character of a compound and, if possible, its structure from IR spectra (various exercises)

NMR spectroscopy: magnetic field, nuclear spin: quantization, I and MI quantum numbers, nuclear magnetic moment, nuclear g-factor, the essence of the nuclear magnetic resonance, Larmor frequency, shielding of nuclei: shielding mechanisms, shielding constant, chemical equivalence of nuclei, the chemical shift, internal standards, the NMR spectrum and its features, NMR spectrometer (demonstration), methodology: the effect of the strength of the magnetic field, integration of a signal, etc., spin-spin coupling, multiplets, <sup>1</sup>H NMR spectroscopy: fundamentals of the method, advantages and disadvantages, <sup>1</sup>H NMR spectrum and its components, electron density and other factors and their influence on the chemical shift (inductive and mesomeric effects etc.), correlation tables, number of signals on the

NMR spectrum: homo-, enantio-, diastereo-, and heterotopic protons (groups of protons), spin-spin coupling constants (determination), magnetic equivalence of the nuclei, the order of the <sup>1</sup>H NMR spectrum, Pople's notation (e.g. AX, AB etc.), roofing effect, dynamic effects and their influence on the <sup>1</sup>H NMR spectrum, virtual coupling, determination of the molecular structure from the <sup>1</sup>H NMR spectra (various exercises), <sup>13</sup>C NMR spectroscopy: fundamentals of the method, proton decoupling (integrated intensities), number of signals on the <sup>13</sup>C NMR spectrum vs. molecular symmetry, shielding of <sup>13</sup>C nuclei, correlation tables, determination of the molecular structure from the <sup>13</sup>C NMR spectra (various exercises)

Electronic spectroscopy: molecular orbital theory – repetition, spectrometers (demonstration) and methodology, types of electronic transitions, selection rules chromophores (various exercises on the intuitive determination of the wavelengths absorbed by different molecules), fluorescence and phosphorescence exercises on the application of electronic spectroscopy in qualitative analysis

Mass spectrometry: Ionization techniques (EI, CI, FAB, FD, MALDI, SIMS etc.), double-focusing (two-sector) mass spectrometer (analyzer), other types of analyzers (quadrupole mass filter, ion trap detector, time of flight analyzer), fragmentation process (the essence, examples, fragmentation of various groups of organic compounds, typical rearrangements), the mass spectrum – types of peaks (ions), relative intensities of the isotope peaks on the mass spectrum, determination and utilization, applications of mass spectrometry in the determination of the molar mass of a molecule and its empirical formula, the nitrogen rule, determination of the molecular structure from the mass spectra (various exercises)

Determination of the molecular structure collectively from the set of IR, NMR and MS spectra – various exercises

#### **Bibliography:**

1. Atkins P. W., Physical Chemistry, Oxford University Press 1994 (or newer).
2. Engel T., Quantum Chemistry and Spectroscopy, Pearson Education, Inc. 2013.
3. Silverstein R. M., Webster F. X., Kiemle D. J., Spectrometric Identification of Organic Compounds, John Wiley and Sons, 2005 (or newer).
4. Lecture notes

All the literature referenced to above is available in the library

#### **Learning outcomes:**

##### KNOWLEDGE

W1. Know the physicochemical fundamentals and basic terms of selected spectral techniques. K\_W15

W2. Know the theoretical fundamentals of the operation of scientific apparatus in the discipline of spectroscopy. K\_W16

##### SKILLS

U1. Be able to interpret the results of research conducted using selected spectroscopic techniques. K\_U1

U2. Be able to read and interpret vibrational, NMR and MS spectra of typical organic compounds. K\_U14

##### ATTITUDES

K1. Know the limitations of his/her knowledge and understand the need of further education and also be able to inspire the learning process in others, in particular in the area of natural sciences. K\_K01

K2. Be able to work in a team and understand the need of teamwork in research in the field of modern chemistry. K\_K02

#### **missing attribute description in English**

Contact hours (work with an academic teacher)

Lecture 15 hrs

Laboratory 30 hrs

Total number of hours with an academic teacher 45

Number of ECTS points with an academic teacher 1.5

Non-contact hours (students' own work)

Preparing to the lab 15 hrs

Literature reading 15 hrs

Preparing to tests 15 hrs

Total number of non-contact hours 45

Number of ECTS points for non-contact hours 1.5

Total number of ECTS points for the module 3

Consultation - 2 hrs

**missing attribute description in English**

W1. lecture – written tests  
W2. lecture, laboratory – written tests  
U1. laboratory – written tests  
U2. laboratory – written tests  
K1. lecture, laboratory – written tests  
K2. laboratory – continuous assessment of students' work

**Requirements**

Fundamentals of physics, physical chemistry and quantum chemistry

**Course credits in various terms:****<without a specific program>**

Type of credits	Number	First term	Last term
European Credit Transfer System (ECTS)	3	14/15L	