Sylabus przedmiotu

Przedmiot:	**Spectroscopy**
Kierunek:	Chemia, II stopień [4 sem], stacjonarny, ogólnoakademicki, rozpoczęty w: 2012
Specjalność:	materials chemistry
Tytuł lub szczegółowa nazwa przedmiotu:	Spectroscopy
Rok/Semestr:	I/2
Liczba godzin:	30,0
Nauczyciel:	**Borowski Piotr, dr hab.**
Forma zajęć:	laboratorium
Rodzaj zaliczenia:	zaliczenie na ocenę
Poziom trudności:	podstawowy
Wstępne wymagania:	fundamentals of physics, physical chemistry and quantum chemistry.
Metody dydaktyczne:	• ćwiczenia przedmiotowe • objaśnienie lub wyjaśnienie • pokaz

Zakres tematów:

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

IR 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
- IR spectrum of a molecule within the harmonic approximation (force constant, selection rules)
- anharmonicity and its effect on the IR 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 IR 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 IR spectrum, group vibrations for various groups of organic compounds (names, notation), correlation tables, hydrogen bonding and its effect on the IR 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 M_I 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
- ^{1}H NMR spectroscopy: fundamentals of the method, advantages and disadvantages, ^{1}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 ^{1}H NMR spectrum, Pople's notation (e.g. AX, AB etc.), roofing effect, dynamic effects and their influence on the ^{1}H NMR spectrum, virtual coupling, determination of the molecular structure from the ^{1}H NMR spectra (various exercises)
- ^{13}C NMR spectroscopy: fundamentals of the method, proton decoupling (integrated intensities), number of signals on the ^{13}C NMR spectrum vs. molecular symmetry, shielding of ^{13}C nuclei, correlation tables, determination of the molecular structure from the ^{13}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*

Forma oceniania:	• ocena ciągła (bieżące przygotowanie do zajęć i aktywność) • śródsemestralne pisemne testy kontrolne
Literatura:	Atkins P. W.,*Physical Chemistry*, Oxford University Press, 1994 (or later) Borowski P.,*Selected problems of Molecular Spectroscopy*, Wydawnictwo UMCS, Lublin 2005. Kęcki Z.,*Fundamentals of Molecular Spectroscopy*, PWN, Warszawa 1998. Sadlej J.,*Molecular Spectroscopy*, WNT, Warszawa 2002. Silverstein R. M., Webster F. X., Kiemle D. J.,*Spectrometric Identification of Organic Compounds*, John WileySons, Inc. New York, 2005