Sylabus przedmiotu

Przedmiot:	**Spectroscopy**
Kierunek:	Chemia, II stopień [4 sem], stacjonarny, ogólnoakademicki, rozpoczęty w: 2013
Specjalność:	materials chemistry
Rok/Semestr:	I/2
Liczba godzin:	15,0
Nauczyciel:	**Patrykiejew Andrzej, prof. dr hab.**
Forma zajęć:	wykład
Rodzaj zaliczenia:	zaliczenie na ocenę
Punkty ECTS:	3,0
Godzinowe ekwiwalenty punktów ECTS (łączna liczba godzin w semestrze):	0 Godziny kontaktowe z prowadzącym zajęcia realizowane w formie konsultacji 0 Godziny kontaktowe z prowadzącym zajęcia realizowane w formie zajęć dydaktycznych 0 Przygotowanie się studenta do zajęć dydaktycznych 0 Przygotowanie się studenta do zaliczeń i/lub egzaminów 0 Studiowanie przez studenta literatury przedmiotu
Poziom trudności:	podstawowy
Wstępne wymagania:	fundamentals of physics, physical chemistry and quantum chemistry
Metody dydaktyczne:	• wykład informacyjny
Zakres tematów:	**Basis of spectroscopy.**Electromagnetic radiation, intensity. Forms of molecular energy. Energy quantization. Spectrum (the origin, classification), experimental techniques (CW, FT – the general ideas), basic apparatus. Selection rules. Band widths. Population of states in thermal equilibrium – Boltzmann distribution. Basis of qualitative and quantitative analysis. **IR 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 IR spectroscopy in the analysis of organic compounds. Hydrogen bonding and its effect on an IR 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 ^{1}H NMR spectroscopy: chemical shifts, the number of signals on the spectrum, the multiplicities of signals. Applications of the ^{1}H NMR spectroscopy in analysis of organic compounds. Hydrogen bonding and its effect on ^{1}HNMR spectrum, dynamical effects in NMR. ^{13}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_2containing 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).
Forma oceniania:	• końcowe zaliczenie pisemne
Literatura:	Atkins P. W.,*Physical Chemistry*, Oxford University Press (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 Identyfication of Organic Compounds*, PWN, Warszawa 2007.