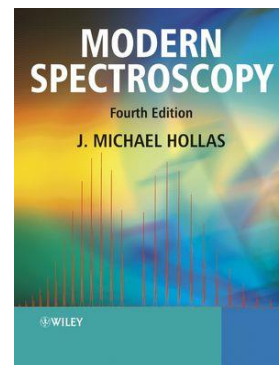
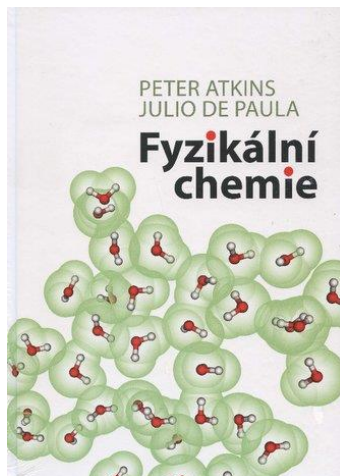
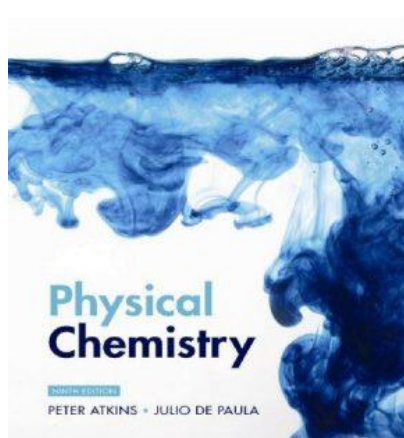


**C9550 Quantum Chemistry and Molecular Spectroscopy**  
**Syllabus - Fall 2019**

- 1. Electromagnetic radiation and its interaction with atoms and molecules**
  - 1.1 Electromagnetic radiation. Hollas 2.1
  - 1.2 Absorption and emission of radiation, line intensity. Hollas 2.2
  - 1.3 Line width. Hollas 2.3
  - 1.4 The electromagnetic spectrum and types of molecular excitations. Hollas 3.1
- 2. Quantum chemical foundations of molecular spectroscopy**
  - 2.1 Principles of quantum mechanics Atkins-EN 7.3-7.7, Atkins-CZ 7.2+7.3
  - 2.2 Selection rules for spectroscopy transitions Atkins-EN 9.3+12.2, Atkins-CZ 9.1.3+12.1.2
- 3. Rotational spectra**
  - 3.1 Rotation in two dimensions: a particle on a ring Atkins-EN 8.6, Atkins-CZ 8.3.1
  - 3.2 Rotation in three dimensions: the particle on a sphere Atkins-EN 8.7, Atkins-CZ 8.3.2
  - 3.3 Moments of inertia Atkins-EN 12.3, Atkins-CZ 12.2.1
  - 3.4 The rotational energy levels Atkins-EN 12.4, Atkins-CZ 12.2.2
  - 3.5 Rotational transitions Atkins-EN 12.5, Atkins-CZ 12.2.3
- 4. Vibrational spectra**
  - 4.1 Harmonic oscillator: the energy levels Atkins-EN 8.4, Atkins-CZ 8.2.1
  - 4.2 Harmonic oscillator: the wavefunctions Atkins-EN 8.5, Atkins-CZ 8.2.2
  - 4.3 Diatomic molecule vibrations Atkins-EN 12.8, Atkins-CZ 12.3.1
  - 4.4 Selection rules Atkins-EN 12.9, Atkins-CZ 12.3.2
  - 4.5 Anharmonicity Atkins-EN 12.10, Atkins-CZ 12.3.3
  - 4.6 Vibration-rotation spectra Atkins-EN 12.11, Atkins-CZ 12.3.4
  - 4.7 Vibration of polyatomic molecules: Normal modes Atkins-EN 12.13, Atkins-CZ 12.4.1
- 5. Electronic spectra**
  - 5.1 The electronic spectra of diatomic molecules Atkins-EN 13.2, Atkins-CZ 13.1.2
  - 5.2 The electronic spectra of polyatomic molecules Atkins-EN 13.3, Atkins-CZ 13.1.3
- 6. The effect of magnetic fields on electrons and nuclei**
  - 6.1 Angular momentum and spin Atkins-EN 8.8, Atkins-CZ 8.3.3
  - 6.2 The spin-orbit coupling Atkins-EN 9.9, Atkins-CZ 9.3.4
  - 6.3 The energies of electrons in magnetic fields Atkins-EN 14.1, Atkins-CZ 14.1.1
  - 6.4 The energies of nuclei in magnetic fields Atkins-EN 14.2, Atkins-CZ 14.1.2
  - 6.5 Magnetic resonance spectroscopy Atkins-EN 14.3, Atkins-CZ 14.1.3
- 7. Electron paramagnetic resonance (EPR) and nuclear magnetic resonance (NMR)**
  - 7.1 EPR g-value and g-tensor Atkins-EN 14.15, Atkins-CZ 14.4.2
  - 7.2 EPR Hyperfine structure Atkins-EN 14.16, Atkins-CZ 14.4.3
  - 7.3 Hyperfine structure – MO relationships for organic radicals Separate study materials
  - 7.4 NMR chemical shift Atkins-EN 14.5, Atkins-CZ 14.2.2
  - 7.5 NMR fine structure Atkins-EN 14.6, Atkins-CZ 14.2.3

## Literature

and its availability in University Kampus Library (on August 23<sup>rd</sup>, 2019)



Atkins' physical chemistry, 9<sup>th</sup> edition, 2010

Fyzikální chemie, překlad 9. vydání, 2013

Modern Spectroscopy, 4<sup>th</sup> edition, 2004

Peter Atkins, Julio de Paula

Peter Atkins, Julio de Paula

J. Michael Hollas

**16 items / 2 loans**

**98 items / 22 loans**

**13 items / 2 loans**

## Class format

Lectures (100 minutes a week, 10 minutes break) and homeworks.

Voluntary assignments will be given to students every week, can be handed in for correction at next lecture.

## Exam

- (1) Written test in Czech or English (on choice). A sample test will be put in IS in the mid-semester at latest. The percent composition: ca 50% of lecture's content and 50% of homework content. 6 pages, maximum 10 points for each. A: 60-54 points, B: 53-48 points, etc.
- (2) Oral part in Czech or English (on choice). 2 pages of the test with the lowest scores will be discussed. Maximum influence of the oral part result on the final grade: Written A or F: no influence. Written B or E: one grade up or down. Written C or D: two grades up or down.