

Hoorcollege

# **Introduction into Spectroscopy**

Autumn semester 2009

Programme:

1. Principles of spectroscopy
2. Transitions between electronic states
3. Rotational & vibrational spectroscopy
4. Electron resonance methods
5. Nuclear magnetic resonance methods

Lecturer: Dr. Jörg Matysik  
Language: English  
Literature: Syllabus  
Doelgroep: 3rd year BSc MST

Further information:

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LCP 101, tel. 4198.

# The programme

## 1 Principles of spectroscopy

### 1.1 Properties of electromagnetic radiation

*Frequency ranges, polarization*

### 1.2 Coupling of electromagnetic radiation to matter

*Absorption, electric dipole transitions, Lambert-Beer law, Kirchhoff's law, Stefan-Boltzmann's law, Wien's displacement law, Rayleigh-Jeans law, Planck law, absorption and emission, Einstein coefficients, scattering, Rayleigh and Mie scattering, refraction, Snell's law, refraction & reflectance, reflection.*

### 1.3 Spectrometers

*Absorption and emission spectrometers.*

### 1.4 Linewidth

*HWHH, Lorentz, Gauss and Voigt.*

## 2 Transitions between electronic states

### 2.1 Electronic transitions of atoms

*Fraunhofer lines, spectral analysis, selection rules, orbital and spin moments, spectrum of hydrogen, term symbols, spin-orbit coupling, Zeeman effect, Stark effect*

### 2.2 Electronic transitions of molecules

*Diatomic molecules, heteronuclear diatomic molecules, selection rules, particle in the box model, types of electronic transitions, vibrational fine structure, Franck-Condon factors, circular dichroism*

### 2.3 Photophysics

*Electronic absorption, fluorescence, phosphorescence, absorption into the continuum, epifluorescence microscopy, principle of a laser*

## 3 Rotational & vibrational spectroscopy

- 3.1 Molecular energy distribution  
*Boltzmann distribution, density of states*
- 3.2 Pure rotational spectra  
*Moment of inertia, selection rules, rotational spectra, rotational Raman effect*
- 3.3 Vibrational spectra  
*Force constant, energy potential, selection rules, band shapes, frequencies, polyatomic molecules, normal modes, vibrational Raman, Resonance Raman*
- 3.4 Spectrometers  
*IR, Raman, dispersive and FT, CARS*
- 3.5 Signal intensities  
*Selection rules, character tables, symmetry*

## 4 Electron resonance methods

- 4.2 Magnetic transitions of electrons  
*Spin, magnetization, magnetic transitions, Zeeman effect in optical spectroscopy and magnetic resonance.*
- 4.3 EPR as method  
*History, mw region, saturation method, stimulated emission.*
- 4.4 A pulsed EPR experiment  
*Classical description, resonance, q-m description, pulse sequence, phase sensitivity, definitions (Polarization, magnetization, relaxation), EPR spectrometer.*
- 4.5 The EPR spectrum  
*Hf-interaction, dipole-dipole interaction, exchange interaction, fine splitting (zero-field splitting), g-value, hf-structure, McConnell equation, electron-nuclear interactions, spin-spin-couplings.*
- 4.6 Special EPR methods  
*Spin probes,  $T_1$  experiments, ENDOR.*

## 5 Nuclear magnetic resonance methods

- 5.1 History and principle  
*History, nuclear spins, nuclear transitions, NMR spectrum, chemical shifts, J couplings, dynamic processes.*
- 5.2 Pulse NMR  
*Pulses, FID, relaxation, correlation time, linewidth,  $T_1$  determination, echo experiments,  $T_2$  determination.*

### 5.3 NMR Techniques

*Gradients, MRI, spin decoupling, nuclear Overhauser effect, 2-dimensional spectroscopy, magic-angle spinning NMR.*

**Last update: 1 Sept. 2009**

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