

Laboratory of Spectroscopy

IR spectroscopy

A dr B. Wrzosek (room 230)

Structural transitions in collagen studied by FT-IR spectroscopy coupled to H/D isotopic exchange

B dr hab. M. Pecul-Kudelska (pok 230)

Determination of the bond length and the magnitude of rotation-oscillation coupling on the basis of the IR spectrum of HCl in gas phase.

Raman spectroscopy

A prof. J. Bukowska (room K, Crystallography)

Characterization of simple aliphatic amides and determination of polypeptide secondary structure by Raman spectroscopy.

B dr A. Królikowska (rooms 301 i 302, Physical Chemistry)

Assignment of CCl₄ molecule normal modes from Raman and IR spectra.

UV-VIS spectroscopy

A prof. J Sadlej /dr hab. M. Pecul-Kudelska

Fluorescence spectroscopy in visible and UV light

B prof. J Sadlej (room 332)

Determination of Dissociation Energy for Iodine Molecule

EPR spectroscopy dr A. Zawadzka-Kazimierczuk (sala 203)

A Reaction of oxidation of hydroquinone and its derivatives

B " "

NMR spectroscopy prof. W. Koźmiński, (kierownik pracowni) (CNBCh 007)

A NMR correlation spectroscopy ,

B Nuclear Overhauser Enhancement,

IR (A)

Structural transitions in collagen studied by FT-IR spectroscopy coupled to H/D isotopic exchange

The exercise is aimed at presenting applications of FT-IR spectroscopy and H/D-exchange in studies on protein structure and stability. Specifically, infrared absorption spectra of H₂O/D₂O mixtures and of thin collagen and gelatin films are acquired and analyzed.

Required knowledge and competences:

Vibrational spectra of molecules

Selection rules for infrared-absorption-induced vibrational transitions

Harmonic and anharmonic oscillators

Effect of isotopic substitution on vibrational bands

Coupling of oscillators and resonance effects

Fermi resonance

Hydrogen bond

Types of secondary structures of proteins

Fourier transform

Protein conformation vs. vibrational bands

H/D-exchange

Collagen and gelatin structure

Sources:

1) Peter Atkins „Physical Chemistry” OUP Oxford

2) Charles R. Cantor and Paul R. Schimmel “Biophysical Chemistry Parts 1, 2, 3” W. H. Freeman

3) Andreas Barth, “Infrared spectroscopy of proteins” *Biochimica et Biophysica Acta (BBA) – Bioenergetics*, Volume 1767, Issue 9, September 2007, Pages 1073–1101

IR (B)

Determination of the bond length and the magnitude of rotation-oscillation coupling on the basis of the IR spectrum of HCl in gas phase,

Requirements:

Types of rotors, quantization of energy, degeneration.

Selection rules for rotational and oscillatory-rotational absorption and Raman spectra.

Rotational structure of absorption spectrum: band positions and intensities.

Rigid rotor and real rotor – comparison of the rotational and oscillatory-rotational spectra.

Reguły wyboru dla przejść absorpcyjnych rotacyjnych i oscylacyjno-rotacyjnych.

Struktura rotacyjna widma oscylacyjnego: położenia i intensywności pasm.

Rotator sztywny i rotator rzeczywisty – porównanie widm rotacyjnych i oscylacyjno-rotacyjnych.

Literature:

1. J. Sadlej „Spektroskopia Molekularna” WNT Warszawa 2002.

2. P.W. Atkins „Physical Chemistry”

3. Materials available from the lab teacher.

UV (A)

Fluorescence spectroscopy in visible and UV light

The objective of this exercise is to familiarize students with the phenomenon of fluorescence and emission/excitation spectra measurements.

The experimental part consists in studying the quenching effect on quinine fluorescence induced by chloride ions. Underlying physical mechanisms, as well as possible practical applications are discussed.

Required knowledge and competences:

Franck-Condon principle

Selection rules for electronic transitions.

Vibrational structure of electronic spectra

Emission electronic spectra: fluorescence and phosphorescence.

Jablonski diagram

Intersystem crossing

Quenching of fluorescence

Sources:

1) Peter Atkins „Physical Chemistry” OUP Oxford

2) Joseph R. Lakowicz “Principles of Fluorescence Spectroscopy” Springer

UV (B)

Determination of Dissociation Energy for Iodine Molecule

Requirement:

Born-Oppenheimer approximation and its consequences;

Potential energy surface (PES) for molecule and the equilibrium geometry;

Dissociation energy and binding energy;

Electronic spectra, selection rules, transition moment, electronic

spectroscopy of diatomic molecules, Franck-Condon principle;

Determination of the Dissociation Energy from electronic spectra.

Bibliography:

1. P.A. Atkins „Physical Chemistry”

2. P.F. Bernath “Spectra of Atoms and Molecules”

Raman spectroscopy (A)

Characterization of simple aliphatic amides and determination of polypeptide secondary structure by Raman spectroscopy

Vibrational spectroscopy. Diatomic harmonic and anharmonic oscillator and

their energy levels. Polyatomic molecules – normal vibrations. Concept of

characteristic vibrations. Vibrational Raman effect – classical and quantum

model of Raman scattering. Selection rules in Raman spectra. Infrared vs.

Raman spectrum. Resonance Raman effect. Raman spectrophotometers (main

elements). Applications of Raman spectroscopy in chemistry and bio-science.

Recommended literature:

P. W. Atkins, Physical Chemistry

Instruction:

1. recording of the Raman spectra of liquid aliphatic amides within a broad range of wavenumbers (500-4500 cm⁻¹)

2. assignment of the observed bands to amide I, II and III and NH stretching vibrations

3. identification of the samples based on discussion of the spectrum and comparison with literature data

4. recording of the Raman spectra of poly(L-glutamic) acid and lysosyme

5. interpretation of the Raman spectra in terms of secondary structure of polypeptides and proteins.

Raman spectroscopy (B)

Assignment of CCl_4 molecule normal modes from Raman and IR spectra

Classes description:

1. Analysis of CCl_4 normal modes using group theory:
 - a) recognition of the point group that studied molecule belongs
 - b) calculating reducible representation and its decomposition into irreducible representations.
 - c) acquiring reducible representation corresponding exclusively to vibrational modes.
 - d) discussion on activity of Raman modes for CCl_4 molecule and polarization properties in Raman spectrum using character table of respective point group
2. Collection of Raman spectrum for liquid CCl_4 (from 150 to 900 cm^{-1}).
3. Collection of polarized Raman modes (for perpendicular and parallel polarization) in a spectral range where Raman bands appear.
4. Collection of a band at 459 cm^{-1} under high resolution conditions.
5. Estimation of depolarization ratios for studied bands and their further application to determine the totally symmetric vibrational mode of CCl_4 .
6. Comparison of similarities and differences between Raman and IR spectrum for CCl_4 .

Description of the results:

1. Exact calculation of the depolarization ratios for given bands
2. Assignment of the Raman components of the band at 459 cm^{-1} to the molecules of different isotopic composition (^{35}Cl and ^{37}Cl)

Natural abundance of isotopes in nature: ^{35}Cl (75.5%) and ^{37}Cl (24.5%)

Entrance test requirements:

Harmonic and anharmonic oscillator (including quantum approach), models of vibrations for multi-atom molecules (terms: internal coordinate, normal coordinate, normal mode, characteristic vibration), electromagnetic radiation scattering, classic theory of Raman scattering, elementary quantum model of Raman spectrum, selection rules for Raman and IR spectrum, polarization of scattered light, depolarization ratio, application of group theory in selection rules determination, block diagram of Raman spectrometer.

EPR (AB)

Reaction of oxidation of hydroquinone and its derivatives

Required material:

Spectrometer EPR, g-factor, organic radicals, hyperfine couplings

Literature:

1. P. Atkins, Atkins' Physical Chemistry
2. <http://nmr.cent3.uw.edu.pl/for-students> 1

NMR (A)

NMR correlation spectroscopy

Basics of NMR: nuclear magnetism, signal detection, Fourier Transformation and its properties, most important spectral parameters, interactions of nuclei in magnetic field, principles of operation of modern NMR spectrometers. Basic application of correlation spectroscopy.

1. P. W. Atkins, Physical Chemistry
2. J. Sanders, Modern NMR Spectroscopy: A Workbook of Chemical Problems

NMR (B)

Nuclear Overhauser Enhancement

Principles of operation of modern NMR spectrometers. Nuclear Overhauser Enhancement

(NOE), applications in chemistry.

1. P. W. Atkins, Physical Chemistry
2. J. Sanders, Modern NMR Spectroscopy: A Workbook of Chemical Problems