Mid-IR spectroscopy

Overview of the entire IR range

- **Near IR** - 12,800 - 4,000 cm⁻¹ (780-2500 μm)
  - Diffuse reflectance: Liquids & solids
  - Transmission: Gases, liquids & solids

- **Mid IR** - (4,000 - 200 cm⁻¹)
  - Transmission: Gases, liquids & solids
  - Diffuse reflectance: Liquids & solids

- **Far IR** - (200 - 10 cm⁻¹)
  - Transmission: Inorganic compounds

Overview

- **Near IR**
  - 12,800 - 4,000 cm⁻¹
  - Transmission: Gases, liquids & solids
  - Diffuse reflectance: Liquids & solids

- **Mid IR**
  - 4,000 - 200 cm⁻¹
  - Transmission: Gases, liquids & solids
  - Diffuse reflectance: Liquids & solids

- **Far IR**
  - 200 - 10 cm⁻¹
  - Transmission: Inorganic compounds

Near IR

- **Diffuse reflectance**
- **Transmission**

Mid IR

- **Transmission**
- **Diffuse reflectance**

Far IR

Light sources in mid-IR

- The Nernst glower
  - 1.200-2.200 K, made of lanthanoid metal oxides

- The Globar glower
  - 1.300-1.500 K, made of silicon carbide

...and maybe in the future

- Quantum Cascade Lasers (QCL:s)
  - QCL:s are built from very narrow semiconductor material → the electrons get trapped and start to behave according to quantum physics

Laser

- A laser creates and amplifies a narrow and intense beam of coherent light
- It requires a metastable excited state
- Population inversion: usually caused by pumping from, for instance, an intense flash of light

Quantum Cascade Lasers

- Each step is producing an electron that in turn can stimulate another electron
  - A QC laser usually consists of 25-75 steps
- High peak power (0.5 W) at room temperature with pulsed lasers
- Wavelength determined by layer thickness rather than by chemical characteristics
  - The whole mid infrared region is covered by the same material
Sample presentation, mid-IR

Gases
   Cells, 1 cm - 10 m (air samples)

Liquids
   Cuvettes with metal halide windows, 0.01 - 1 mm

Solids
   Tablets of KBr
   Nujol techniques

Solvents for mid-IR

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<th>Wavenumber, cm⁻¹</th>
<th>5000</th>
<th>2500</th>
<th>1667</th>
<th>1250</th>
<th>1000</th>
<th>833</th>
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Wavelength, μm

2  4  6  8  10  12  14  16

Lines indicate useful regions

Mid-IR

Infrared spectroscopy on biological systems is usually performed in transmission mode.

This means that the IR beam of the spectrometer is passing through the sample and the transmitted IR intensity is measured.

Owing to the high IR absorptivity of water, IR samples are very thin, usually only a few micrometer optical pathlength.

ATR

In this technique, the IR beam is guided in an IR transparent crystal by total reflection. Due to quantum mechanical properties of the IR light, the electromagnetic field may extend beyond the crystal surface for about one micron as a so-called evanescent field.
Micro-ATR unit which have ZnSe light guide optics and a thin diamond or Silicon ATR plate with only 4 mm diameter.

Detectors, mid-IR

Thermal detectors
Blackbody in vacuum, temperature measurement

Thermo-element
Two different metals, voltage measurement at various temperatures of the two metals

Bolometers
Semiconductor thermistor

Pyroelectric detectors
Single crystals of a pyroelectrical material. The crystal is polarized in a electrical field. The capacitance is temperature dependent.
Sufficiently rapid response for FTIR-instruments.

Photoelectrical detectors
IR-sensitive semiconductor material, most common is the mercury/cadmium telluride (MCT) detector.
Operates at 77K (liquid nitrogen) to minimize thermal noise.
Sufficiently rapid for FTIR-instruments.
A typical IR spectrum

Group frequency interpretation

Group frequency interpretation

Group frequency interpretation

Computer based identification

chloroform
deuterochloroform
General rule, IR

The greater the masses of attached atoms, the lower the IR frequency at which the bond will absorb

mid-IR spectroscopy

– not only for identification!
Today it is also a quantitative technique
Dedicated instruments are now on the market

MilkoScan™ FT120

MilkoScan™ FT 120 employs the FTIR measuring principle, in compliance with IDF and AOAC standards. A complete analysis of product composition with up to 24 parameters can be presented in just 30 seconds. MilkoScan FT 120 is suitable for both process control and sophisticated analysis in the lab. The basic configuration offers determination of fat, protein, lactose, total solids and solids-non-fat in milk, cream and simple dairy products.

WineScan FT 120

With WineScan FT 120, all major parameters can be determined in one single analysis. In 30 seconds you have an accurate measurement of, for example: Ethanol, total acid, volatile acid, malic acid, pH, lactic acid, glucose, fructose and reducing sugar without using reagents.