Infrared and Raman spectroscopy

Sir C.V. Raman - Nobel prize for physics 1930

Why are these methods important for medical applications?

Vibration modes of water molecules

http://www1.lsbu.ac.uk/water/vibrat.html
Energy system of molecules

- high energy: excited states
- low energy: ground state
- vibrational levels
- rotational levels
- electronic levels
- excited states

How to use this information to characterize molecules?

Simple considerations: a spring.

Model for molecular vibrations

- spring = bond
- mass = atom

\[ f \sim \frac{D}{m} \]

if \( m_{\text{mass}} \) ↑ then \( f \) ↓

- (C-H: 3000 cm\(^{-1}\), C-Cl: 700 cm\(^{-1}\))

if bond strength ↑ then \( f \) ↑

- (C-H: 1650 cm\(^{-1}\), C≡C: 2200 cm\(^{-1}\))

What is elastic and non-elastic scattering?

Infra and Raman spectroscopy

Infra spectroscopy: how can the substance absorb infrared light.

Raman spectroscopy: how can the substance scatter infrared light?
Advantages of Raman spectroscopy

• works on a wide range of concentrations: from 100% to ppb (parts per billion)
• spectra are recorded within a couple of seconds
• qualitative and quantitative analysis (width/area of peaks depends on quantity, proportion of components can be calculated)
• works even through walls of plastic or glass containers

www.medschool.pte.hu

Example: IR spectrum

x-axis: wavelength (wavenumber)
typically 2.5-15 µm (4000-600 cm⁻¹)
y-axis: usually transmittance (0 - 100%) (valleys correspond to absorption)

Example: regions of an IR spectrum

Bonds to H (5 - 16) 
(4000-2500 cm⁻¹) 
Triple bonds 
(2500-2000) 
Double bonds 
(2000-1500) 
"Fingerprint" region 
(1500 - 600)

Example: IR spectrum analysis

The spectrum seems to be consistent with a compound containing a carbonyl group and only saturated CH. The carbonyl band is at 1760 cm⁻¹, suggestive of an ester linkage. The band at 1250 cm⁻¹ is consistent with a CO bond.

Summary

- molecular vibrations;
- energy transitions;
- Raman scattering;
- applications.
Thank you!