Raman Spectroscopy

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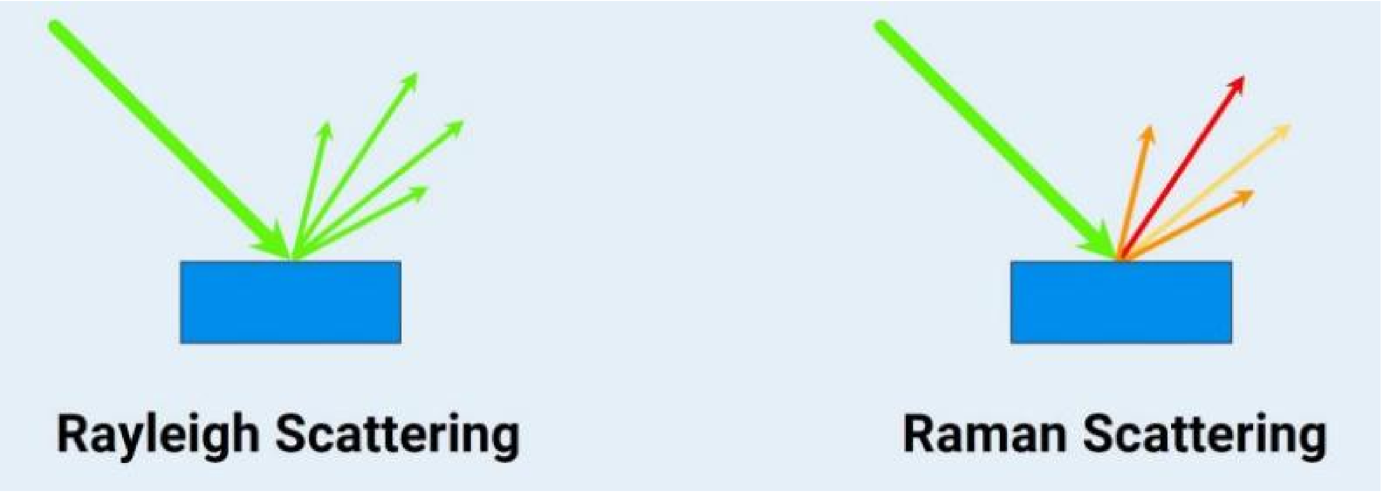
https://www.bruker.com/en/products-and-solutions/infrared-and-raman/raman-spectrometers/what-is-raman-spectroscopy.html

What is Raman spectroscopy?

- Raman spectroscopy is a chemical analysis technique which involves illuminating a substance with a laser and analyzing the light that is scattered off the surface of the substance. The scattered light can provide a lot of information about the substance and its structure, and can be used to identify, characterize, and quantify many chemical components.

Light scattering?

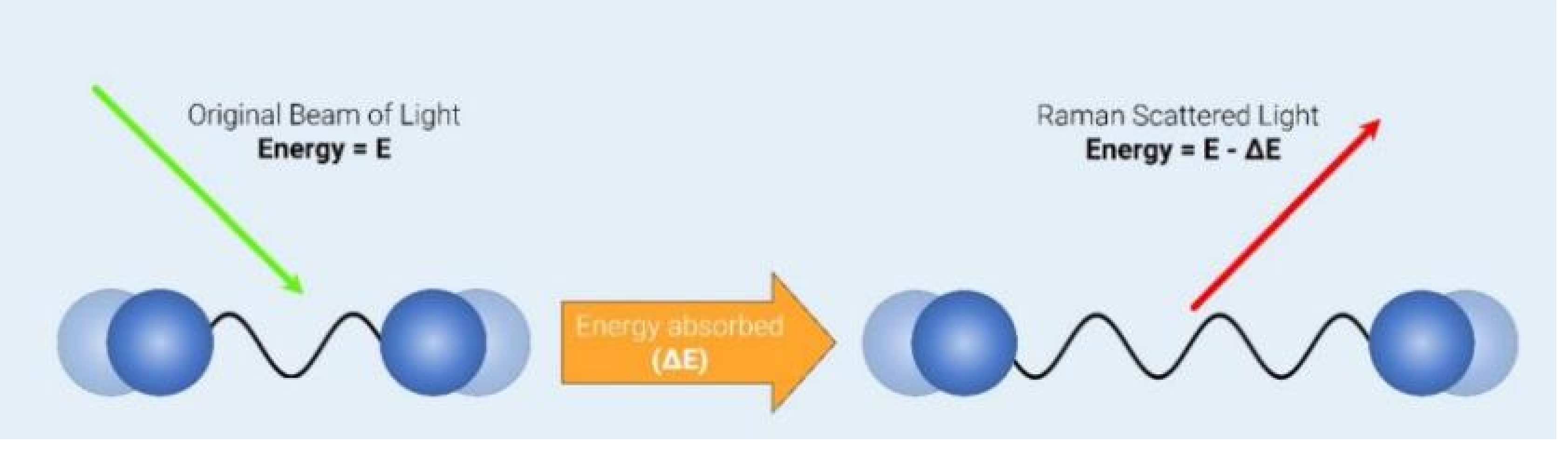
- When light is scattered off a sample there are two possible outcomes:
- **(1) Elastic scattering**, also known as Rayleigh scattering, occurs when the scattered light has the same energy as the light that initially struck the sample. This means that the elastically scattered light will be the same frequency, wavelength, and color as the original beam of light.
- **(2)** Inelastic scattering, or **Raman scattering**, occurs when the scattered light has a different energy than the light that initially struck the sample. This means the inelastically scattered light will have a different frequency, wavelength, and color than the original beam of light.



The Raman effect

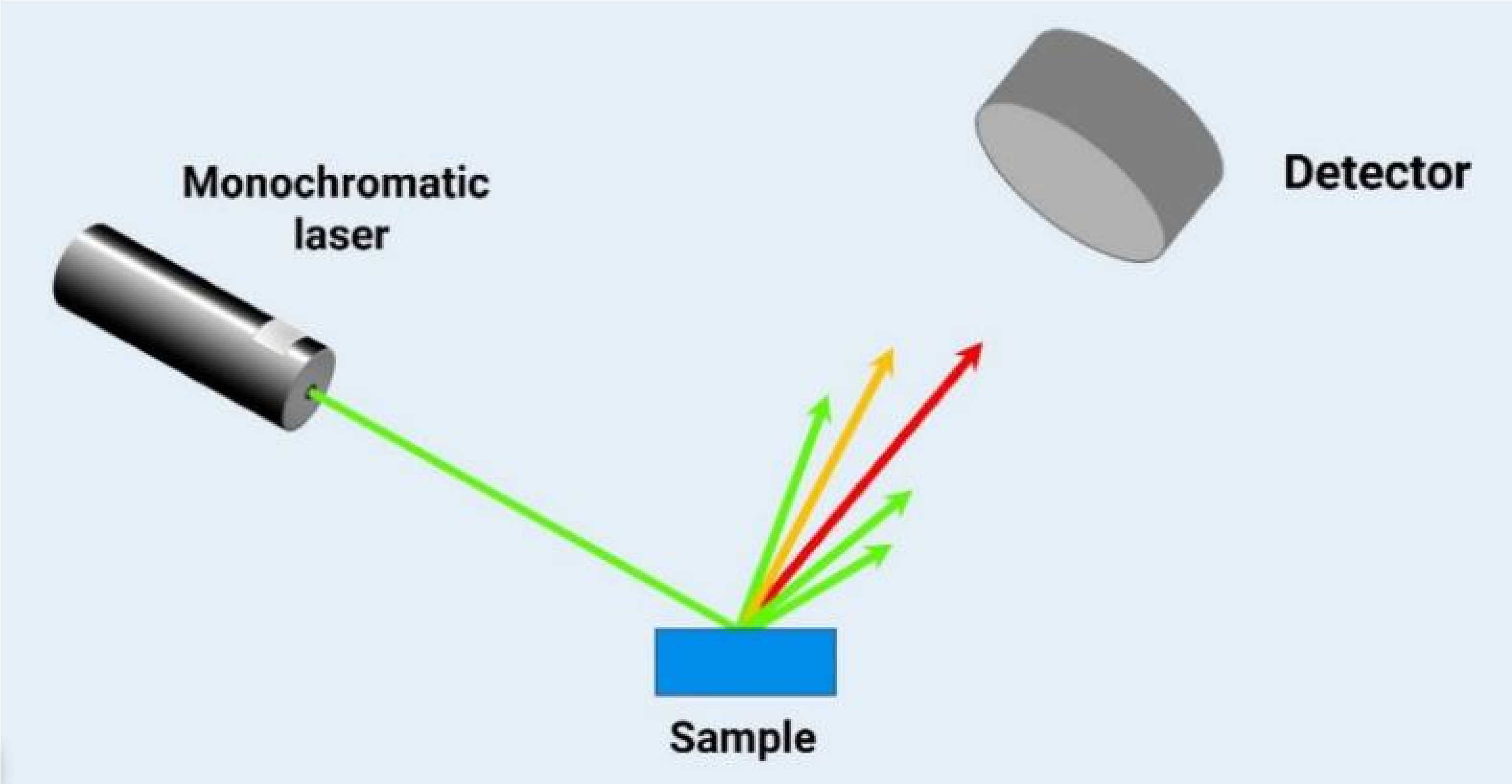
- The constant motion of atoms in a molecule, which makes the bonds in atoms kind of like springs are constantly vibrating in different directions.
- These molecular vibrations happen at specific frequencies which are unique to the molecule and type of bond.
- An popular and easy example for such a spring is molecular oxygen (O_2) or nitrogen (N_2).
- We typically discuss the vibrational frequencies of molecules in terms of wavenumbers, which have units of reciprocal centimeters [cm^{-1}].
- So for example, oxygen gas in our atmosphere vibrates at around 1550 cm^{-1}, while nitrogen gas vibrates at 2330 cm^{-1}.
- Larger molecules with lots of chemical bonds will have **many different molecular vibrations** occurring at different frequencies.

- Now, every time incoming light has the same frequency as the vibration of the molecule, light can be absorbed, "exciting" the vibration further, and amplifying its amplitude.
- Since the different bonds in molecules vibrate at different frequencies, different molecules will absorb unique frequencies of light to excite vibrations.
- If a molecule is illuminated with light, the molecule may absorb **some of that light** to excite a molecular vibration.
- If that happens, the light that scatters off the molecule will come back at a different frequency and color since some of the light from the original beam was absorbed by the molecule.
- This phenomenon is called the Raman effect, and it's the cause of Raman scattering.



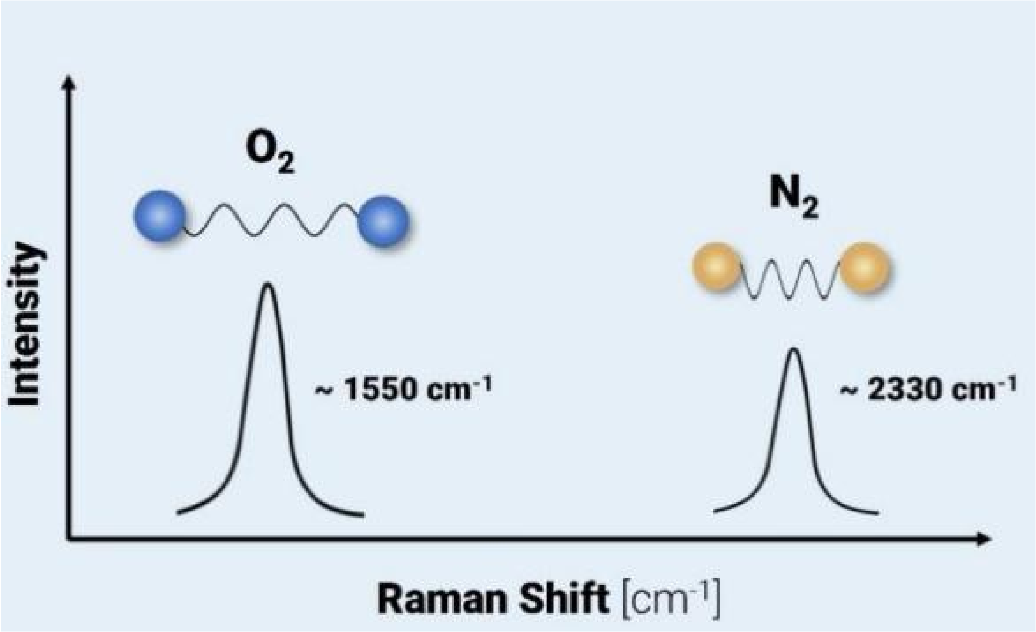
Raman spectroscopy

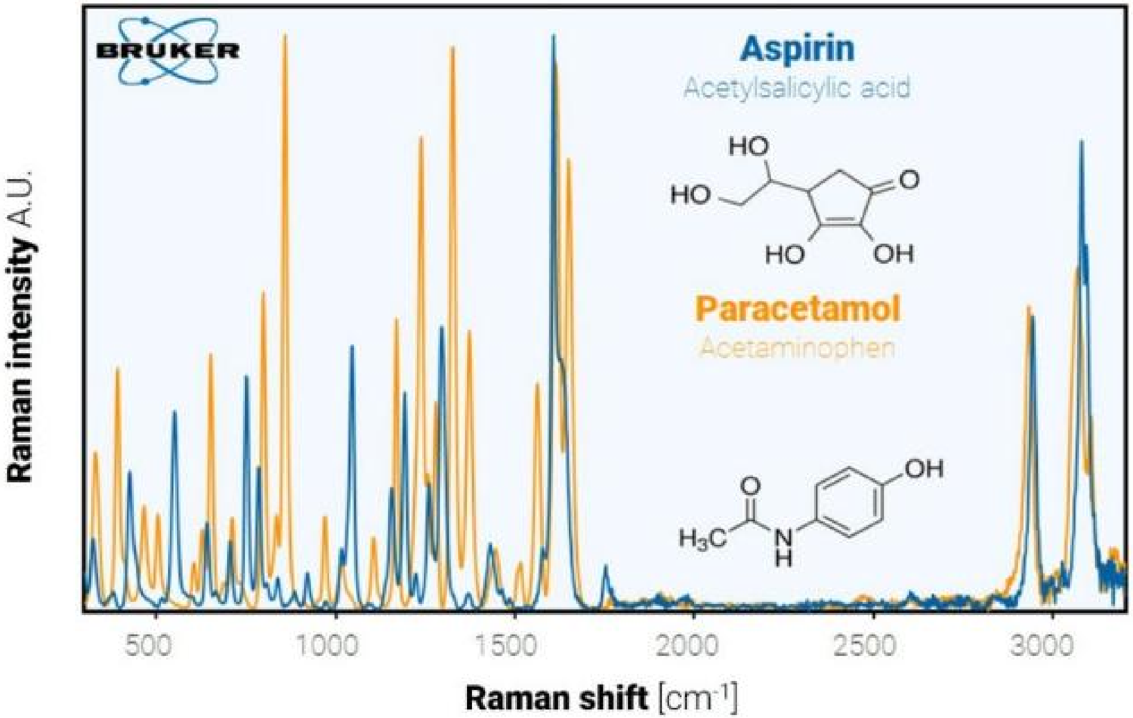
- Since the frequencies of light absorbed when a molecule is illuminated are unique to the molecule and type of bonds, detecting these frequencies of light will allow us to figure out which molecules are present in the sample.
- This is the aim of Raman spectroscopy.
- When those molecules absorb some of the light (inelastic scattering), the frequency of the light changes.
- So to detect the Raman effect, we can simply determine **the frequency shift** between the original beam of light and the Raman scattered light.
- The frequency shift is called the Raman shift.
- By using a monochromatic laser for the experiment we can easily determine the frequency of the original light beam, since lasers emit light that is all the same wavelength and frequency.
- The typical choice is a green laser (532 nm).
- To make it clear: When the sample is illuminated with the laser, some of the laser light will be absorbed by the sample to excite molecular vibrations, causing Raman scattering.
- The Raman scattered light is then collected at a detector so we can determine its frequency.
- That will give us all the information we need to determine the Raman shift.


Monochromatic
laser
Detector
Sample

Raman spectrum

- Once we know the Raman shifts, we can plot that information to create the Raman spectrum.
- Each peak on the Raman spectrum corresponds with a different frequency of light absorbed by the sample which excited a vibration.
- Since these frequencies are unique to the molecule and the types of bonds it contains, the Raman spectra creates a "chemical fingerprint" that allows us to identify and quantify a large variety of substances.
- For example, we know oxygen vibrates at around 1550 cm^{-1} while nitrogen vibrates at 2330 cm^{-1}.
- If we illuminate these gases with our green laser, the gases will absorb those frequencies of light which we'll see on the Raman spectra.
- There will be a peak for oxygen around 1550 cm^{-1} and a peak for nitrogen around 2330 cm^{-1}.
- Many molecules are quite complex, containing many chemical bonds with lots of different molecular vibrations.
- So, the Raman spectrum for most molecules will contain many peaks.
- Luckily, the Raman spectra of many compounds have already been measured and compiled into vast spectral libraries.
- Computer software can compare measurements against these spectral libraries for effortless identification of nearly any sample.


O2
N2
Intensity
~ 1550 cm-1
~ 2330 cm-1
Raman Shift [cm-1]


BRUKER
Aspirin
Acetylsalicylic acid
HO
HO
O
HO
OH
Paracetamol
Acetaminophen
OH
O
H3C
N
H
Raman intensity A.U.
500
1000
1500
2000
2500
3000
Raman shift [cm-1]