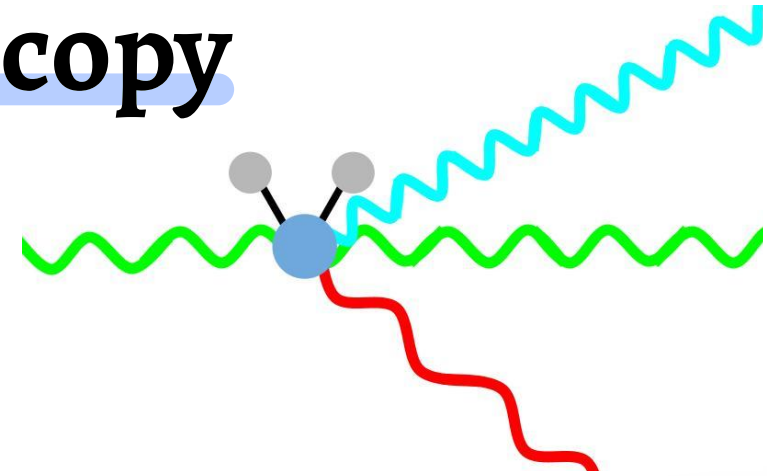
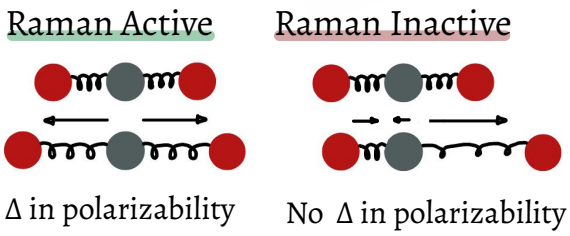
Raman Spectroscopy



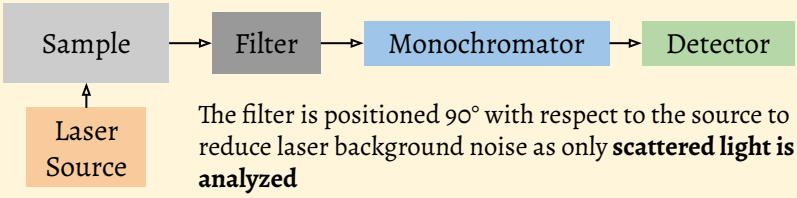
Summary

Raman spectroscopy is commonly used to **measure vibrational modes** of molecules with the goal of qualitative **structure identification**. Raman spec takes advantage of how species of molecules have different **vibrational energy levels** in order to identify bonds. Depending on the strength of a bond, the atoms involved, and the surrounding atoms, bonds will **vibrate at quantized energies**. These specific energies can be measured by exciting the molecule with a laser and recording the raman scattering that occurs.

What Makes a Vibration Raman Active?
The molecule must undergo a change (Δ) in polarizability. **Polarizability** describes the ease of distorting electrons from their original position.



Instrumentation



The filter is positioned 90° with respect to the source to reduce laser background noise as only **scattered light is analyzed**

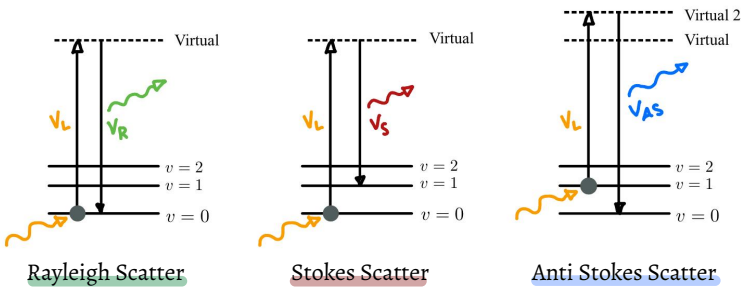
Source: Monochromatic laser light (single or few λ)
Sample: liquid or solid, gas cannot be used
Filter: filters out laser light and lets scattered light through
Monochromator: separates light in selectable wavelengths
Detector: Detects photons and sends signals to readout device

Limitations

- **Raman scattering is very rare** and the Raman scattered light signal is weak compared to Rayleigh scattering
- Many compounds are not Raman active
- Fluorescence can often overwhelm a Raman signal
- Glass and microslides can mask Raman signal
- Vessels and substrates can be included in the Raman signal
- The **laser λ must not be on analyte absorption band** as to avoid Rayleigh peak covering Raman peaks

Theory

Monochromatic laser light is used to excite the sample molecule to a virtual energy state. The molecule stays at this virtual state for a very short time and relaxes down to either the ground vibration state (v=0) or a higher vibrational state (v=1). The relaxation emits light at the frequency corresponding to the energy difference of relaxation.



The **energy difference** of the ground state vibration (v=0) and the (v=1) vibrational state is calculated and used to identify the type of bond present in the sample.

Stokes: $V_S = V_L - V_{0->1}$
Anti stokes: $V_{AS} = V_L + V_{0->1}$

Applications

Qualitative
Species identification/structure determination. Using the fingerprint spectra, analytes can be determined by comparing spectra to other known compound spectra (similar to IR spectra)
Drug or active ingredient determination: It is often used to test for presence of illegal drugs. This test does not harm or use up the sample.

Quantitative
Concentration determination: The peak intensity directly correlates with the number of bonds in the sample. A standard curve can be used to measure unknown analyte concentration.