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Time: 10: 00 am

MPHYCC10 Atomic and Molecular Physics

# Raman Spectroscopy

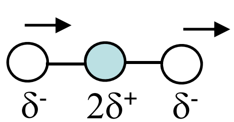
## *A) Introduction*

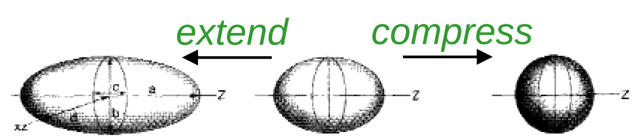
1.) Raman spectroscopy: *complementary to IR spectroscopy*.

- radiation at a certain frequency is scattered by the molecule with *shifts* in the wavelength of the incident beam.
- observed frequency shifts are related to vibrational changes in the molecule → associated with IR absorbance.
- Raman Scattering Spectrum Resembles IR absorbance spectrum
- Raman & IR mechanism differ

a) comparison of Raman & IR:

| IR | Raman |
|---|---|
| i. vibrational modes | vibrational modes |
| ii. change in dipole | change in polarizability |

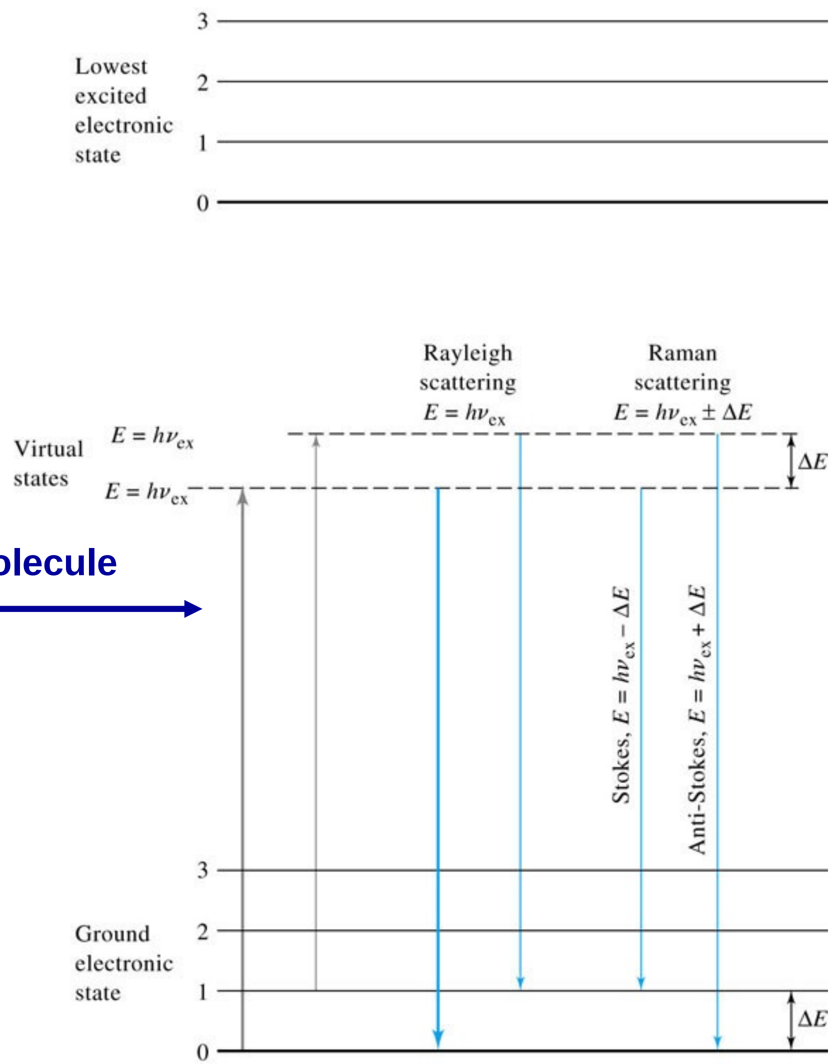



| IR | Raman |
|---|---|
| iii. excitation of molecule to excited vibrational state | momentary distortion of the electrons distributed around the bond |
| iv. asymmetric vibrations (active) | symmetric vibrations (active) |

2.) Basic Principals of Raman Spectroscopy:

- light is scattered by the sample at various angles by momentary absorption to virtual state and reemission



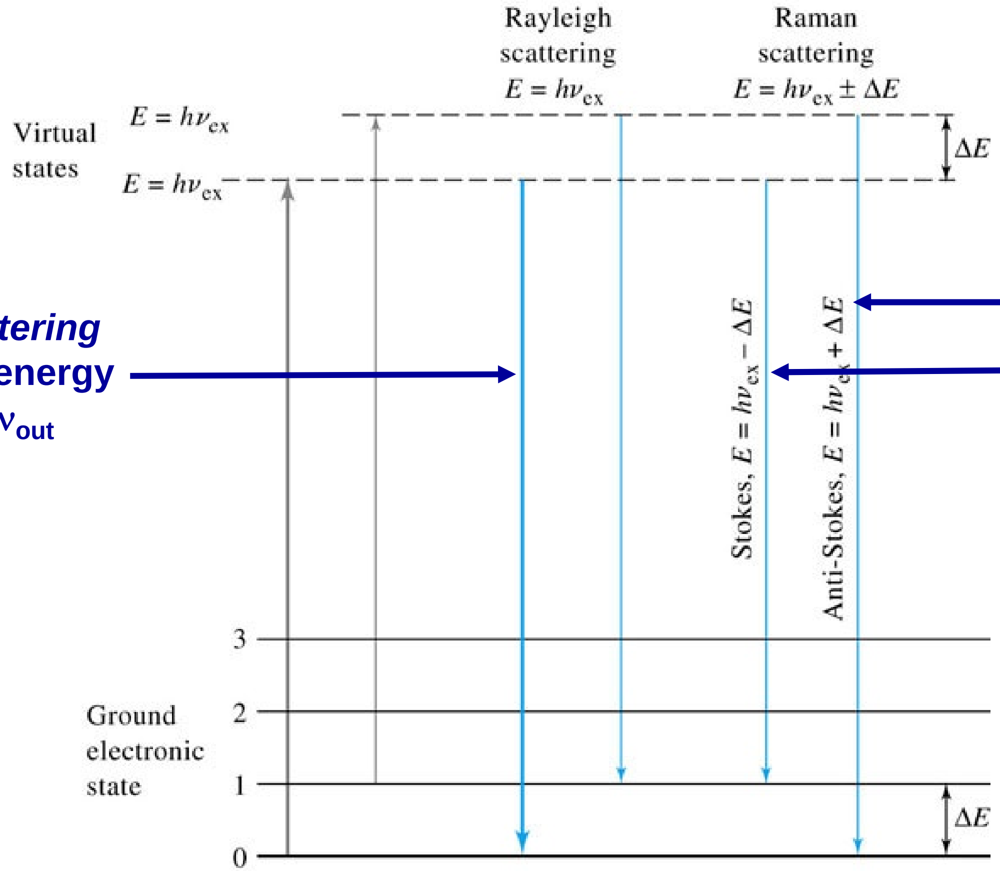

No change in electronic states

Infinite number of virtual states

**energy absorbed by molecule from photon of light** → ***not quantized***

- some scattered emissions occur at the same energy while others return in a different state

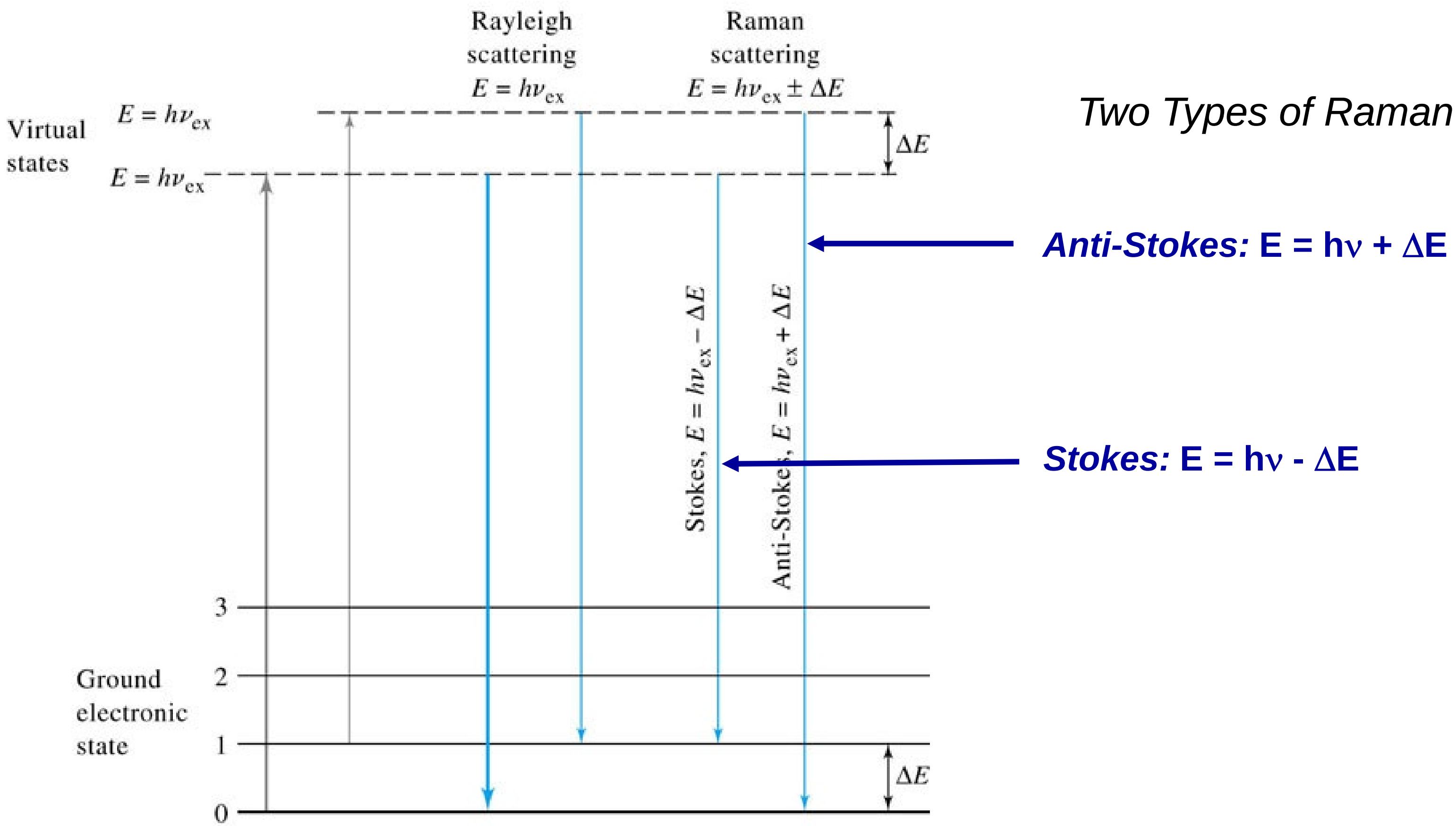
***Rayleigh Scattering***
**no change in energy**
**$h\nu_{in} = h\nu_{out}$**




***Raman Scattering***
**net change in energy**
**$h\nu_{in} <> h\nu_{out}$**

<u>Elastic</u>: collision between photon and molecule results in no change in energy
<u>Inelastic</u>: collision between photon and molecule results in a net change in energy

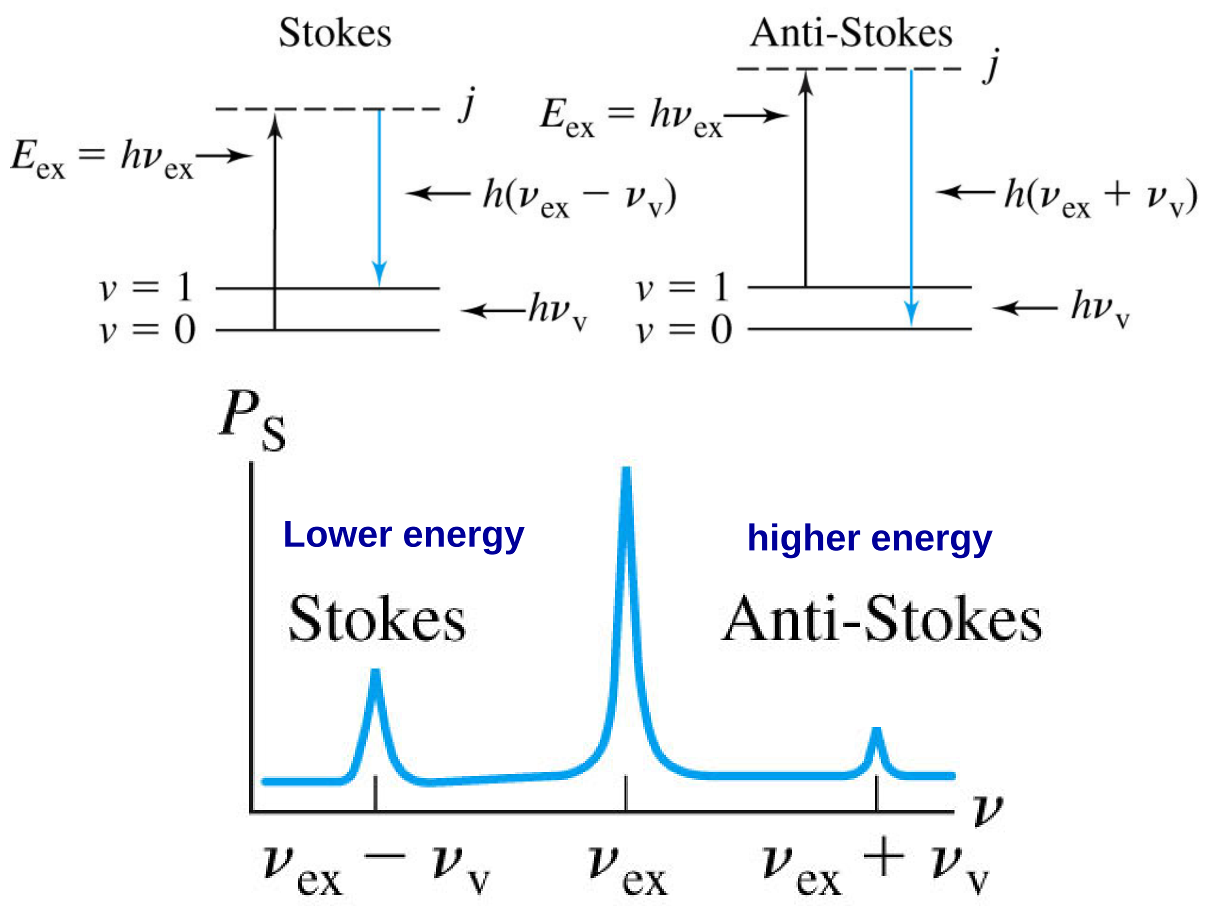
## *Two Types of Raman Scattering*




±ΔE – the energy of the first vibration level of the ground state – *<u>IR vibration absorbance</u>*

∴ Raman *frequency shift* and IR absorption *peak frequency* are *identical*

## - Resulting Raman Spectrum




Probability of Emission $\propto$ Observed Intensity

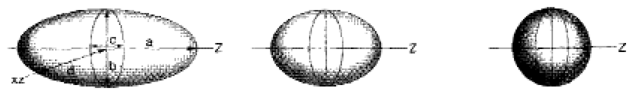
Raleigh scattering >> Stokes >> anti-Stokes

difference in population of energy levels of vibrational transitions

*Intensity of Raman lines are 0.001% intensity of the source*

3.) Active Raman Vibrations:

- need change in polarizability of molecule during vibration
- polarizability related to electron cloud distribution



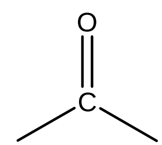
example:

O = C = O — IR inactive, Raman active

O = C = O — IR active, Raman inactive

*IR & Raman are complimentary*. Can be cases where vibration is both IR & Raman active (eg. $SO_2$ – non-linear molecule)

In general:

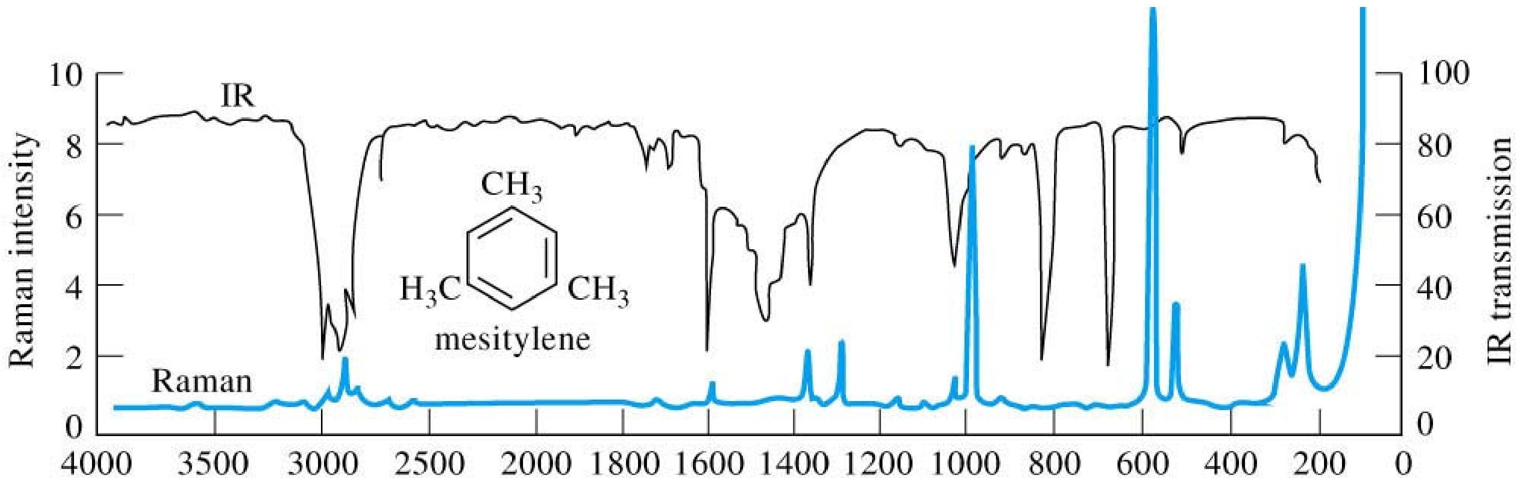
IR tends to emphasize polar functional groups (R-OH,  , etc.)

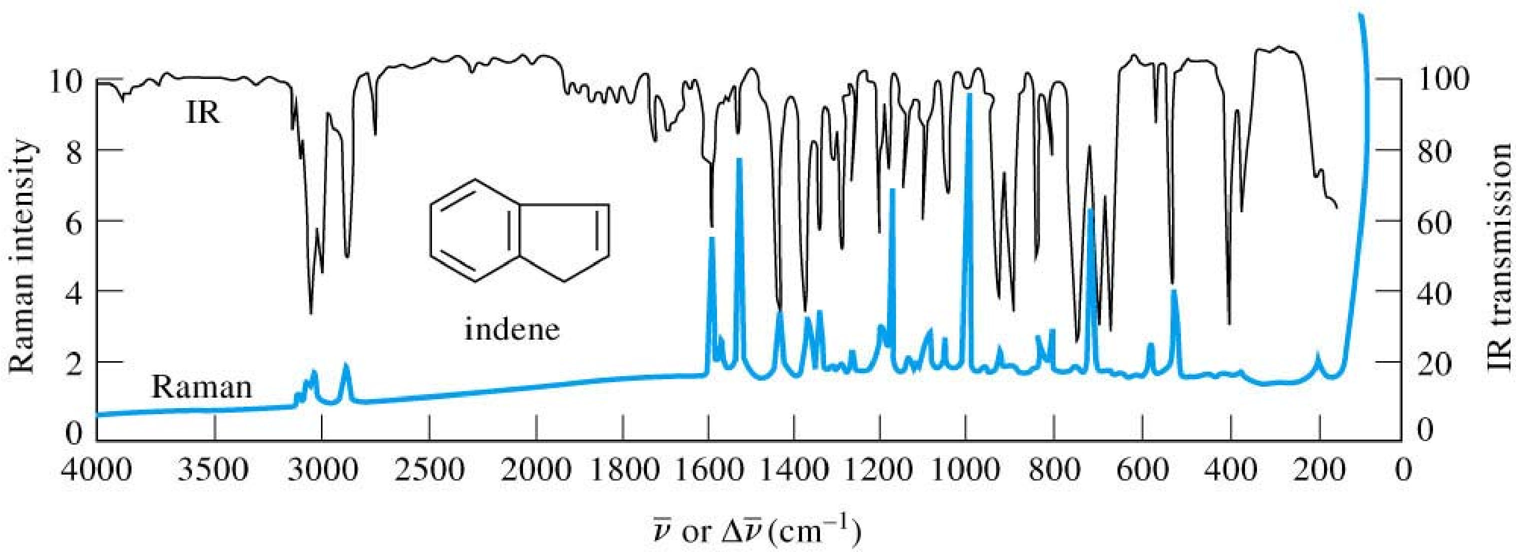
Raman emphasizes aromatic & carbon backbone (C=C, -$CH_2$-, etc.)

- Raman does not "see" many common polar solvents can use with aqueous samples – advantage over IR

*Raman frequency range*: 4000 -50 $cm^{-1}$(Stokes and anti-stokes)

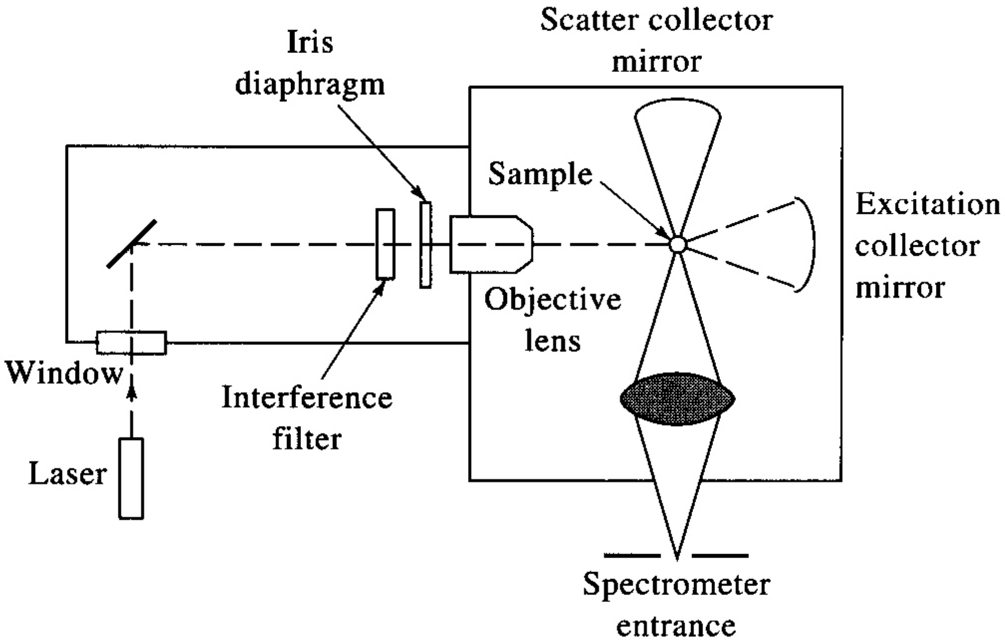
- comparison of Raman and IR Spectra



4.) Instrumentation:

- Basic design




i. ) *Light source*:

- generally a laser to get required intensity of light for reasonable S/N
    - Raman scattering is only 0.001% of light source
- Doesn't have to be in IR region, since look at changes around central peak.
    - visible source used because of high intensity
    - allows use of glass/quartz sample cells & optics
    - UV/Vis type detectors (photomultiplier tubes)

4.) Applications:

a) Qualitative Information

i. characteristic regions for different groups as in IR
ii. Raman correlation charts available
iii. Good for aqueous based samples
iv. Useful for a variety of samples, organic, inorganic & biological

b) Quantitative Information – *not routinely used*

i. fewer technical problems than IR, fewer peaks
ii. Interference from fluorescence
iii. Higher cost
iii. Signal weak – require modified Raman methods

1) Resonance Raman spectroscopy allows detection of $10^{-3}$ ->$10^{-7}$M by using lasers light with wavelength approaching *electronic* absorption
2) Surface enhanced Raman spectroscopy places samples on metal or rough surfaces that increase Raman scattering