

# IR & Fourier Transform IR

By-Dr.Wagh J.G.

Dept.Pharmaceutical Chemistry

MES COLLEGE OF PHARMACY

SONAI

# Introduction

- ▶ Spectroscopy is an analytical technique which helps to determine the structure of the compounds.
- ▶ It destroys little or no sample.
- ▶ The amount of light absorbed by the sample is measured as wavelength is varied.

# Infrared Spectroscopy

It Provides information about the vibrations of functional groups in a molecule

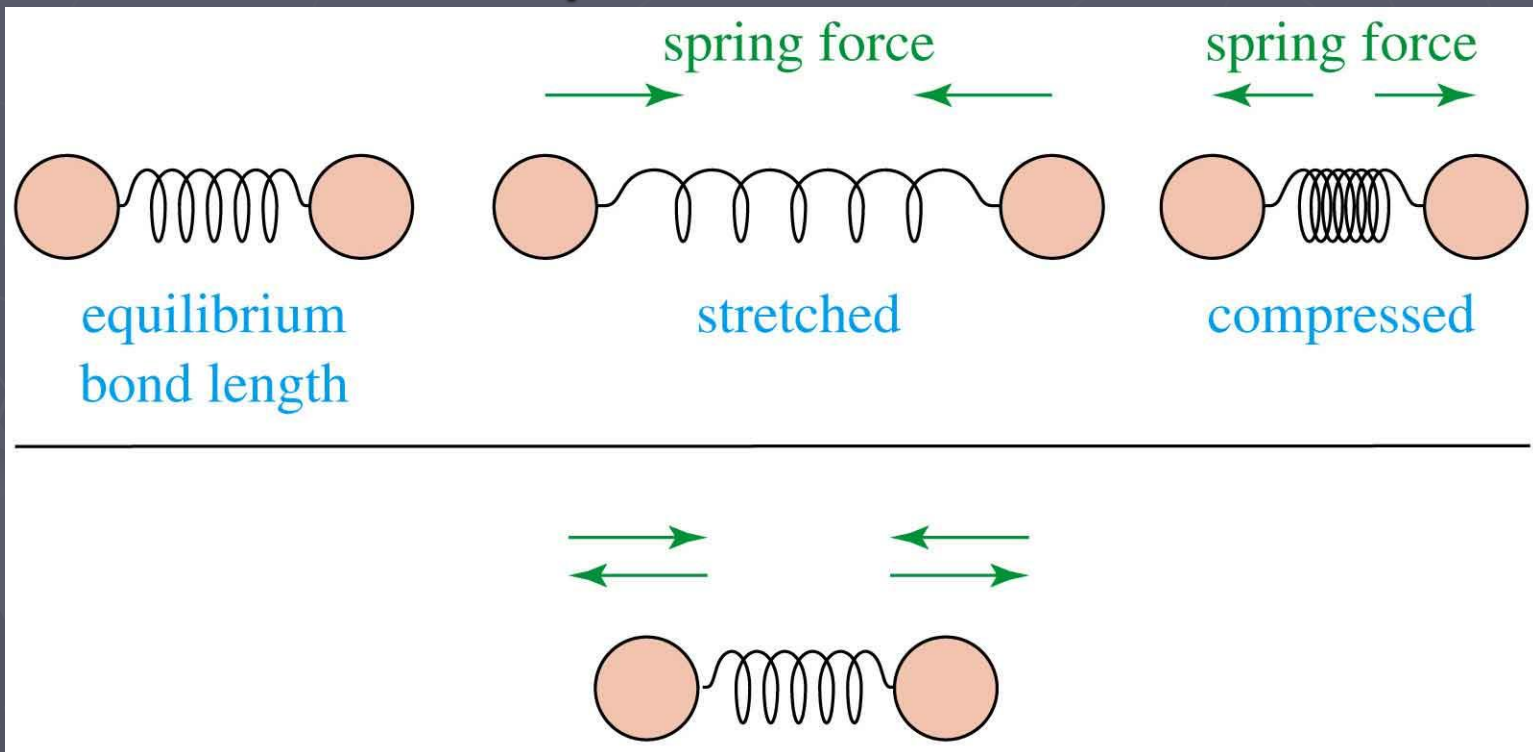
Therefore, the functional groups present in a molecule can be deduced from an IR spectrum

# The IR Region

- ▶ Just below the red in the visible region usually between the range of 2.5 - 25  $\mu\text{m}$ .
- ▶ More common units are wave numbers, or  $\text{cm}^{-1}$ , the reciprocal of the wavelength in centimeters.

# Molecular Vibrations

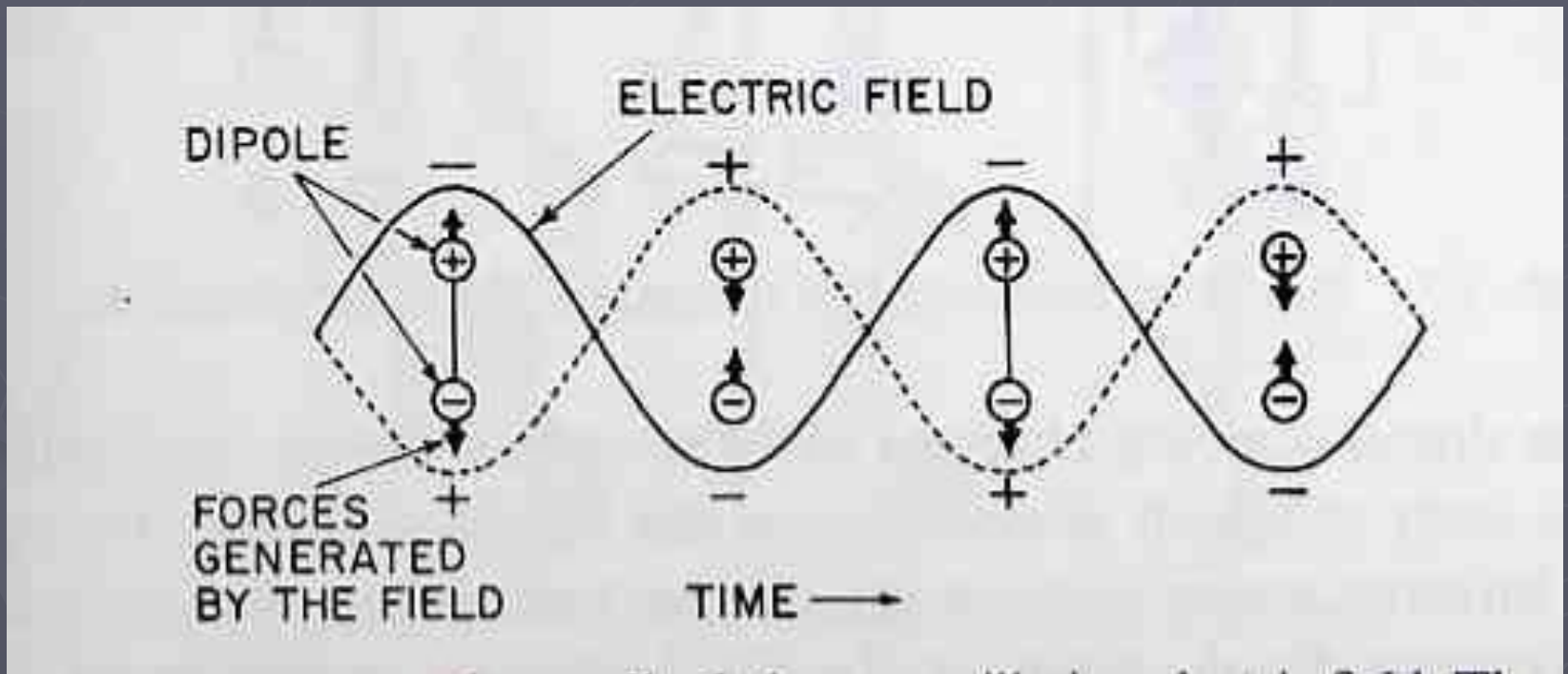
Covalent bonds vibrate at only certain allowable frequencies.



# IR: Masses, Atoms and Springs

A Model: Picture the atoms of a diatomic molecule as point masses connected by springs (bonds).

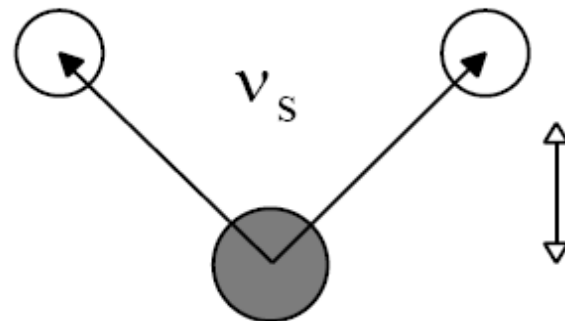
The greater the **change** in dipole moment during a vibration, the higher the intensity of absorption of a photon



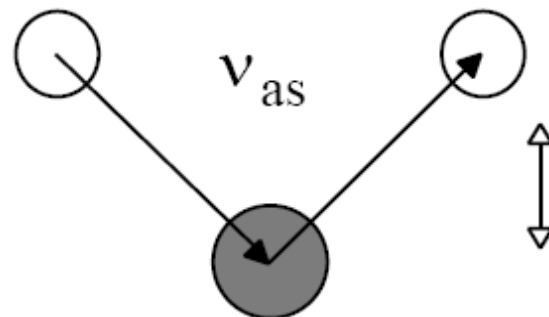
### iii.) Types of Molecular Vibrations

#### Bond Stretching

*symmetric*



*asymmetric*





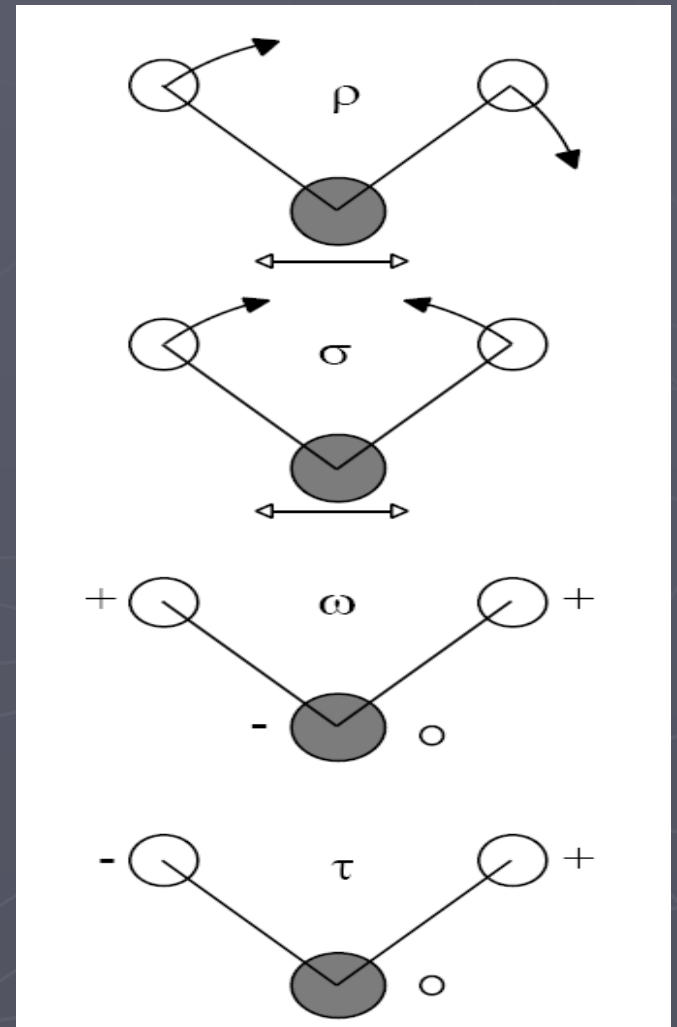
# Bond Bending

*In-plane rocking*

*In-plane scissoring*

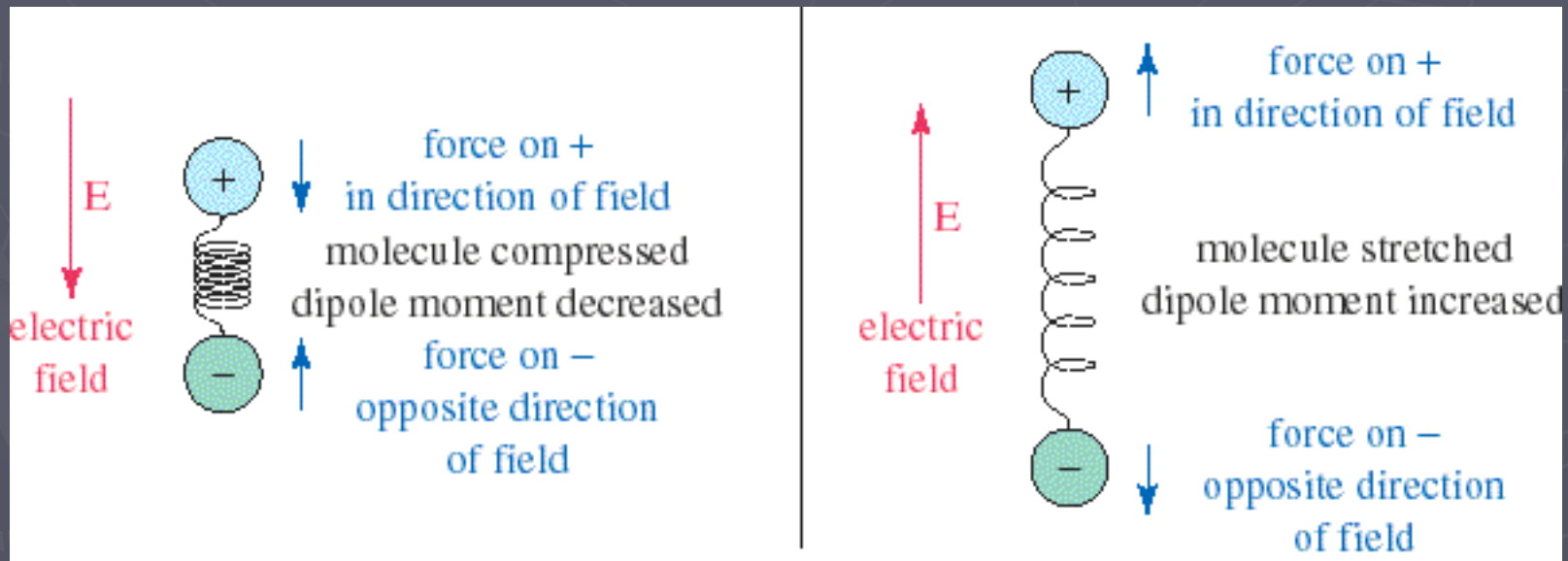
*Out-of-plane wagging*

*Out-of-plane twisting*



# IR-Active and Inactive

- ▶ A polar bond is usually IR-active.
- ▶ A nonpolar bond in a symmetrical molecule will absorb weakly or not at all.



# FTIR Instruments Components

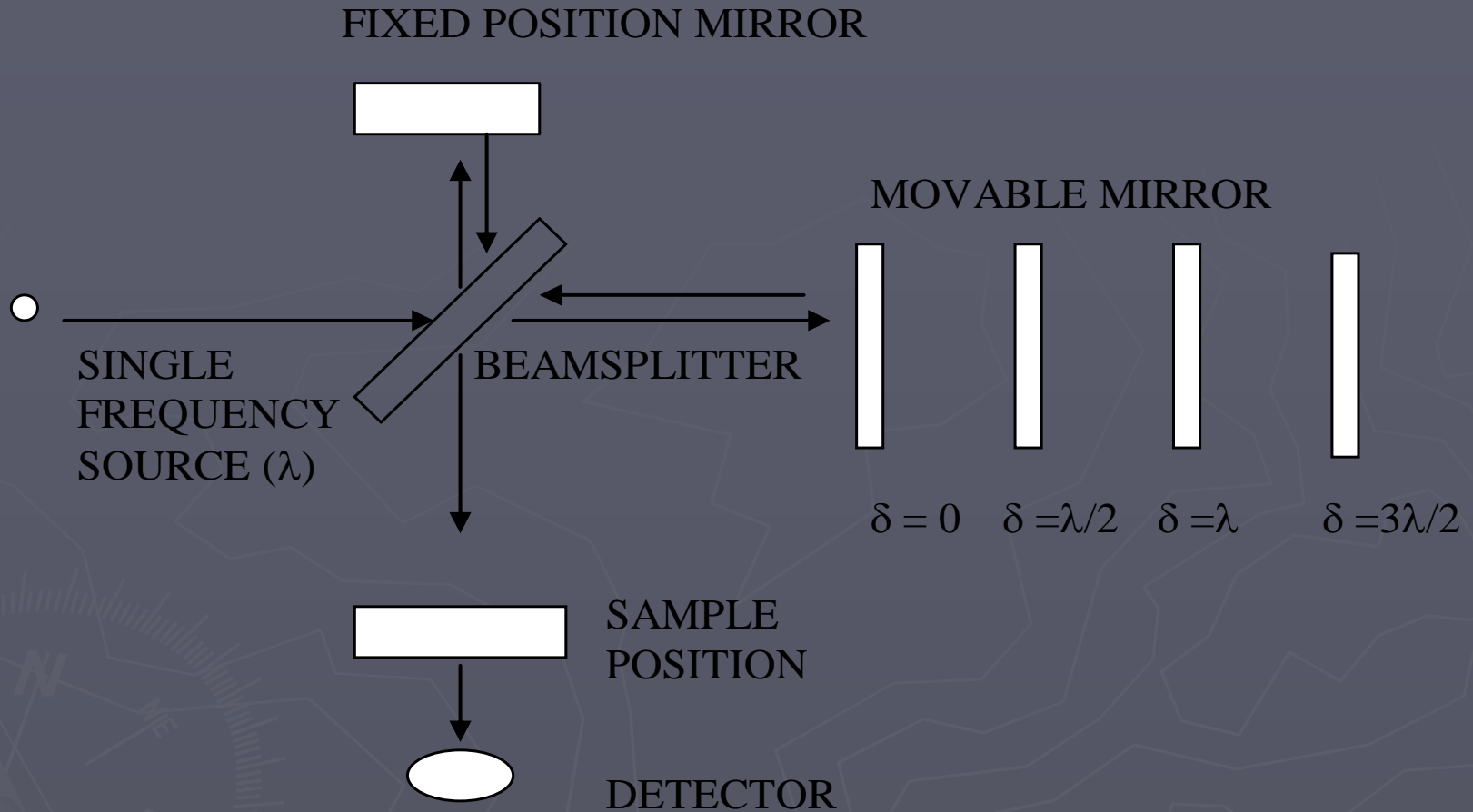
- ▶ Source
- ▶ Michelson Interferometer
- ▶ Sample
- ▶ Detector

# Sources

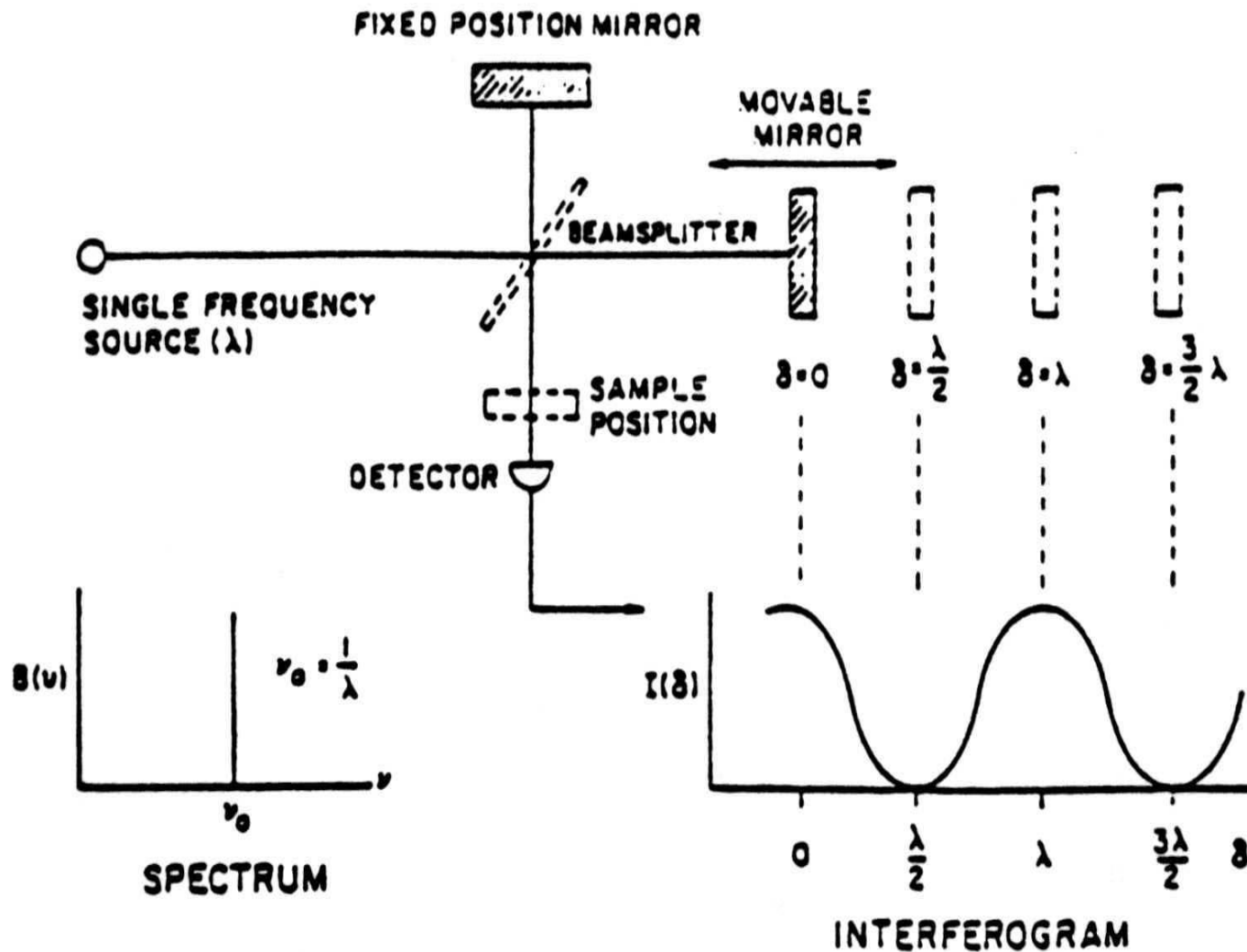
- ▶ Black body radiators
- ▶ Inert solids resistively heated to 1500-2200 K
- ▶ Max radiation between 5000-5900  $\text{cm}^{-1}$  (2-1.7  $\mu\text{m}$ ), falls off to about 1 % max at 670  $\text{cm}^{-1}$  (15  $\mu\text{m}$ )
- ▶ Nernst Glower – cylinder made of rare earth elements
- ▶ Globar- SiC rod
- ▶  $\text{CO}_2$  laser
- ▶ Hg arc (Far IR), Tungsten filament (Near IR)

# Michaelson Interferometer

- ▶ Beam splitter
- ▶ Stationary mirror
- ▶ Moving mirror at constant velocity
- ▶ He/Ne laser; sampling interval, control mirror velocity



# THE MICHELSON INTERFEROMETER



Schematic of a Michelson Interferometer.

# Sample

- ▶ Sample holder must be transparent to IR- salts
- ▶ Liquids
  - Salt Plates
  - Neat, 1 drop
  - Samples dissolved in volatile solvents- 0.1-10%
- ▶ Solids
  - KBr pellets
  - Mulling (dispersions)



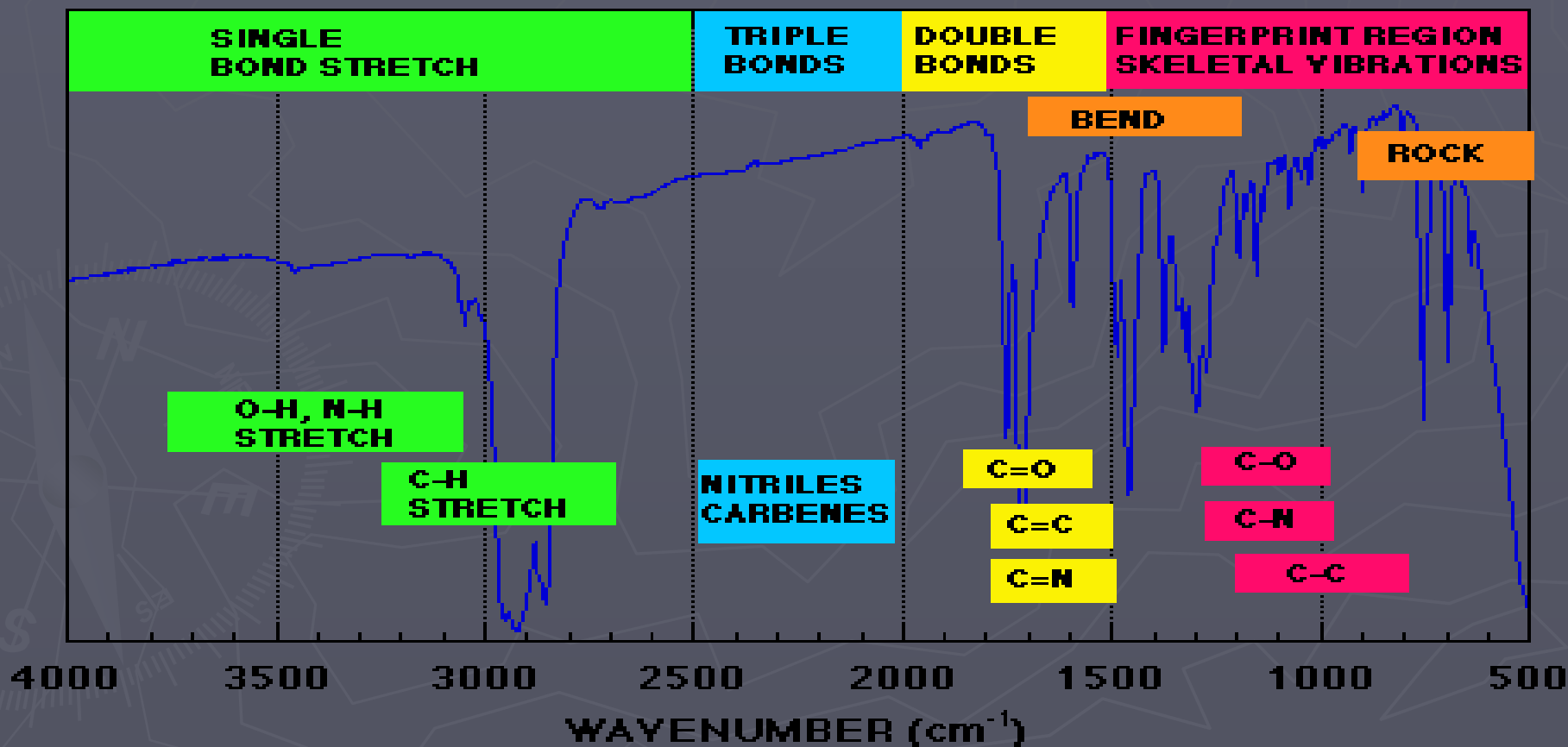
# FT-IR detectors

- ▶ Pyroelectric transducers (PTs)
- ▶ Pyroelectric substances act as temperature-dependent capacitors
- ▶ Triglycine sulfate is sandwiched between two electrodes. One electrode is IR transparent
- ▶ The current across the electrodes is Temperature dependent
- ▶ PTs exhibit fast response times, which is why most FT instruments use them

## Advantages of FTIR compared to Normal IR:

- 1) much faster, seconds vs. minutes
- 2) use signal averaging to increase signal-to-noise (S/N)
- 3) higher inherent S/N – no slits, less optical equipment, higher light intensity
- 4) high resolution ( $<0.1 \text{ cm}^{-1}$ )

1) Examine what functional groups are present by looking at group frequency region - 3600  $\text{cm}^{-1}$  to 1200  $\text{cm}^{-1}$



THANK YOU

