

IR & Fourier Transform IR

By-Dr.Wagh J.G.

Dept.Pharmaceutical Chemistry

MES COLLEGE OF PHARMACY

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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

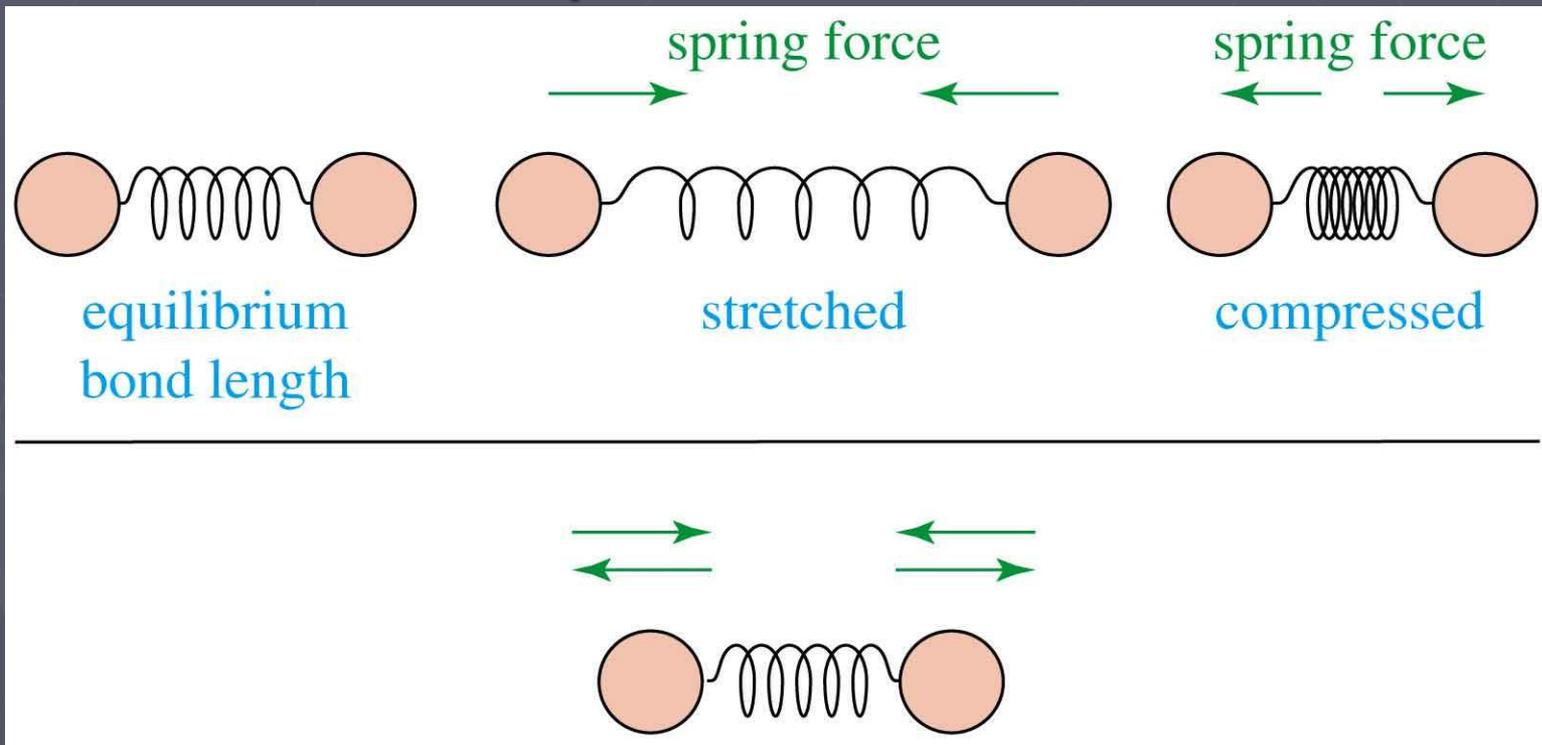
Therefore, the functional groups present in a molecule can be deduced from an IR spectrum

The IR Region

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

Molecular Vibrations

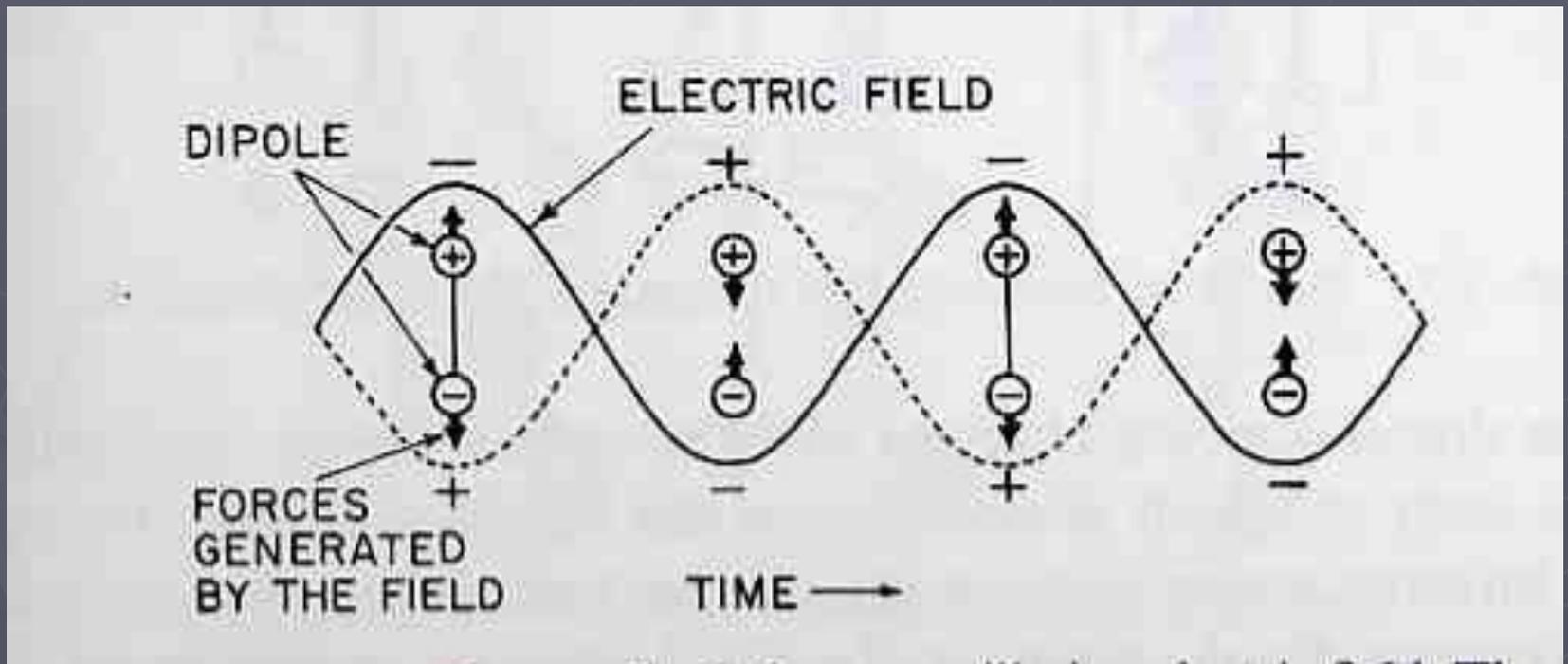
Covalent bonds vibrate at only certain allowable frequencies.



IR: Masses, Atoms and Springs

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

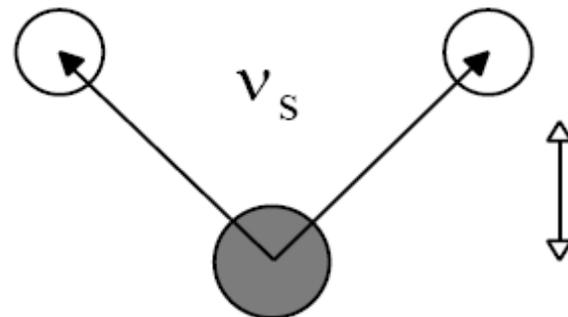
The greater the **change** in dipole moment during a vibration, the higher the intensity of absorption of a photon



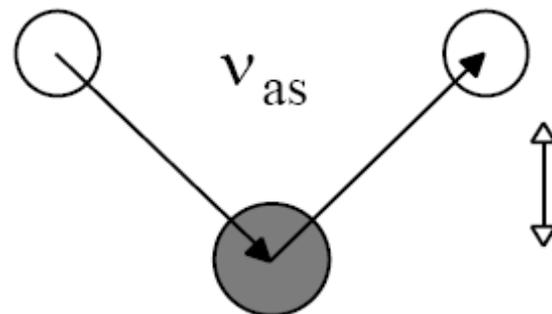
iii.) Types of Molecular Vibrations

Bond Stretching

symmetric



asymmetric



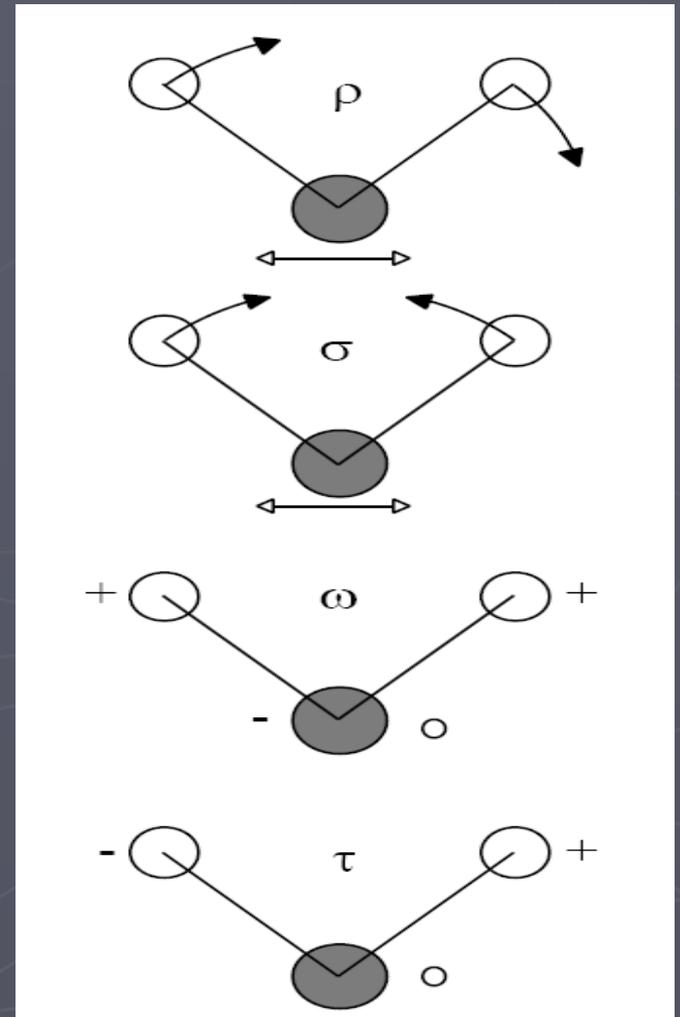
Bond Bending

In-plane rocking

In-plane scissoring

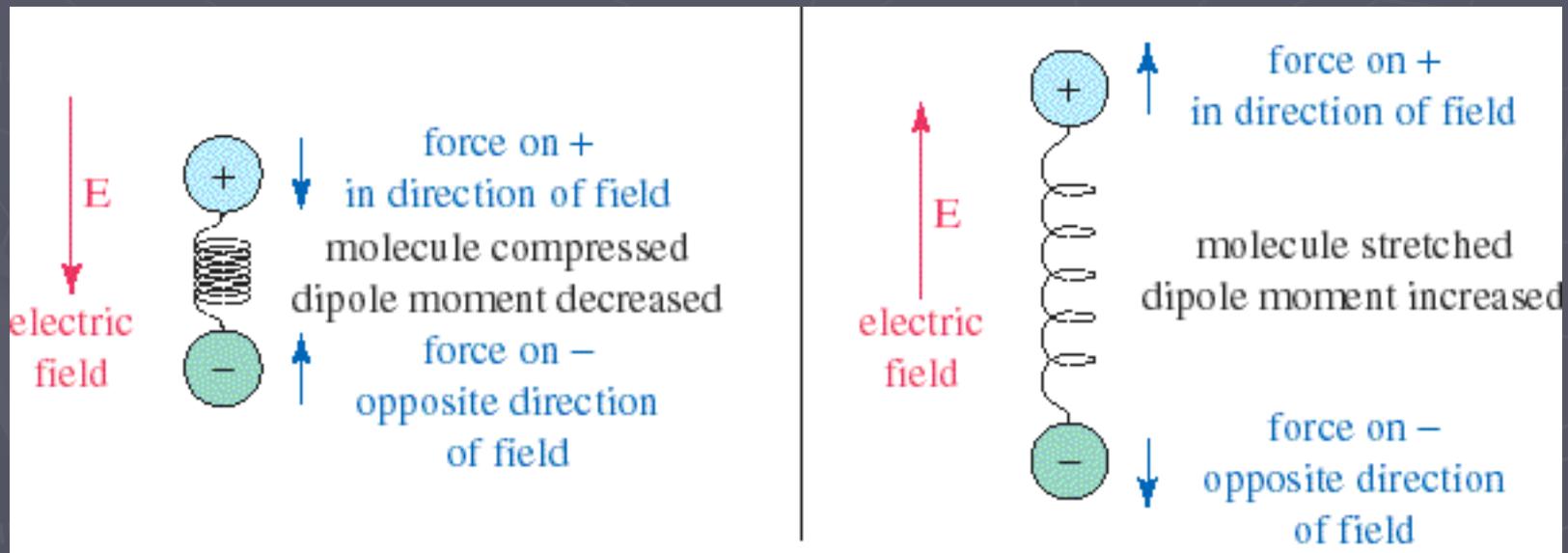
Out-of-plane wagging

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

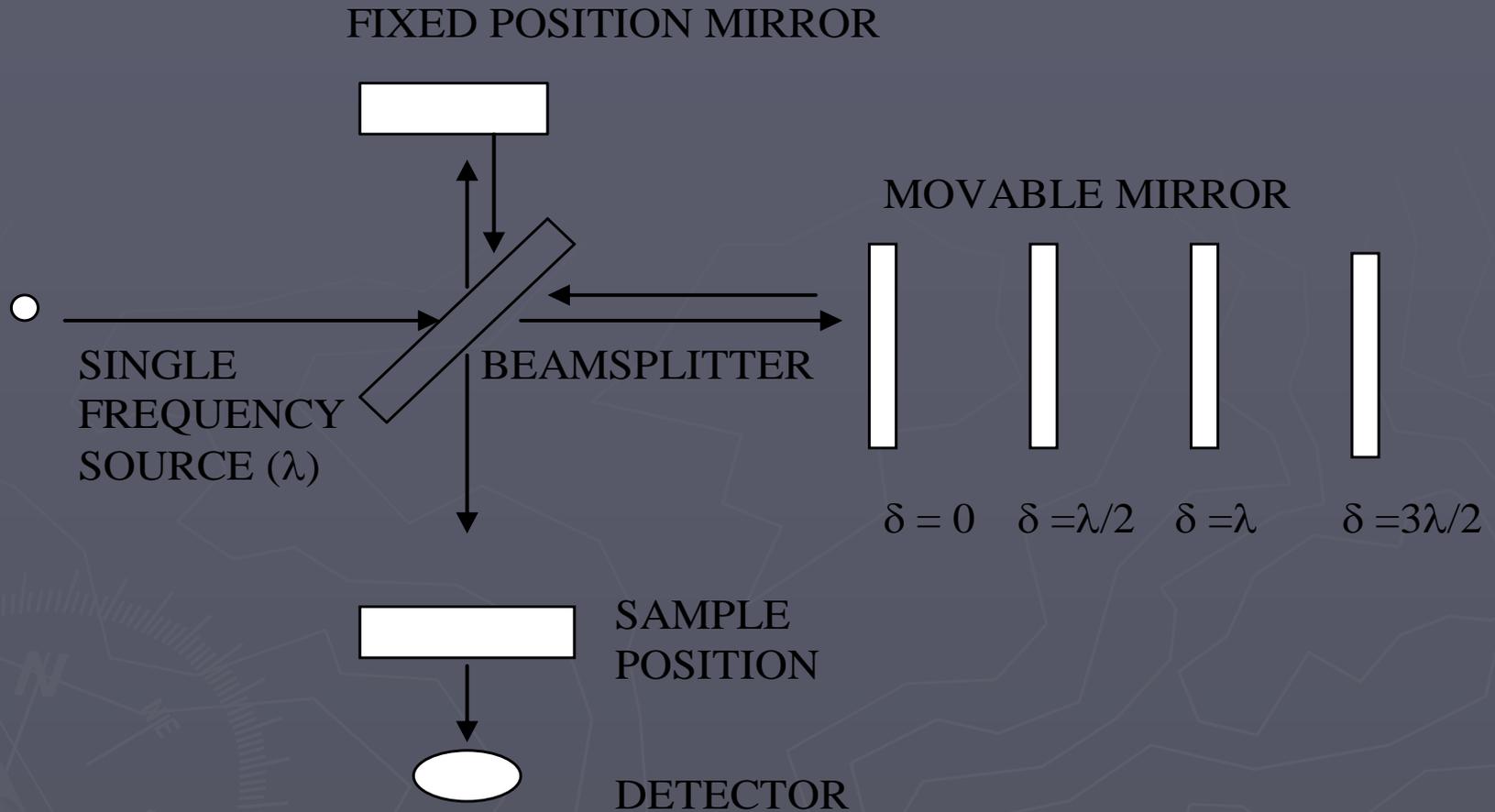
- ▶ Source
- ▶ Michelson Interferometer
- ▶ Sample
- ▶ Detector

Sources

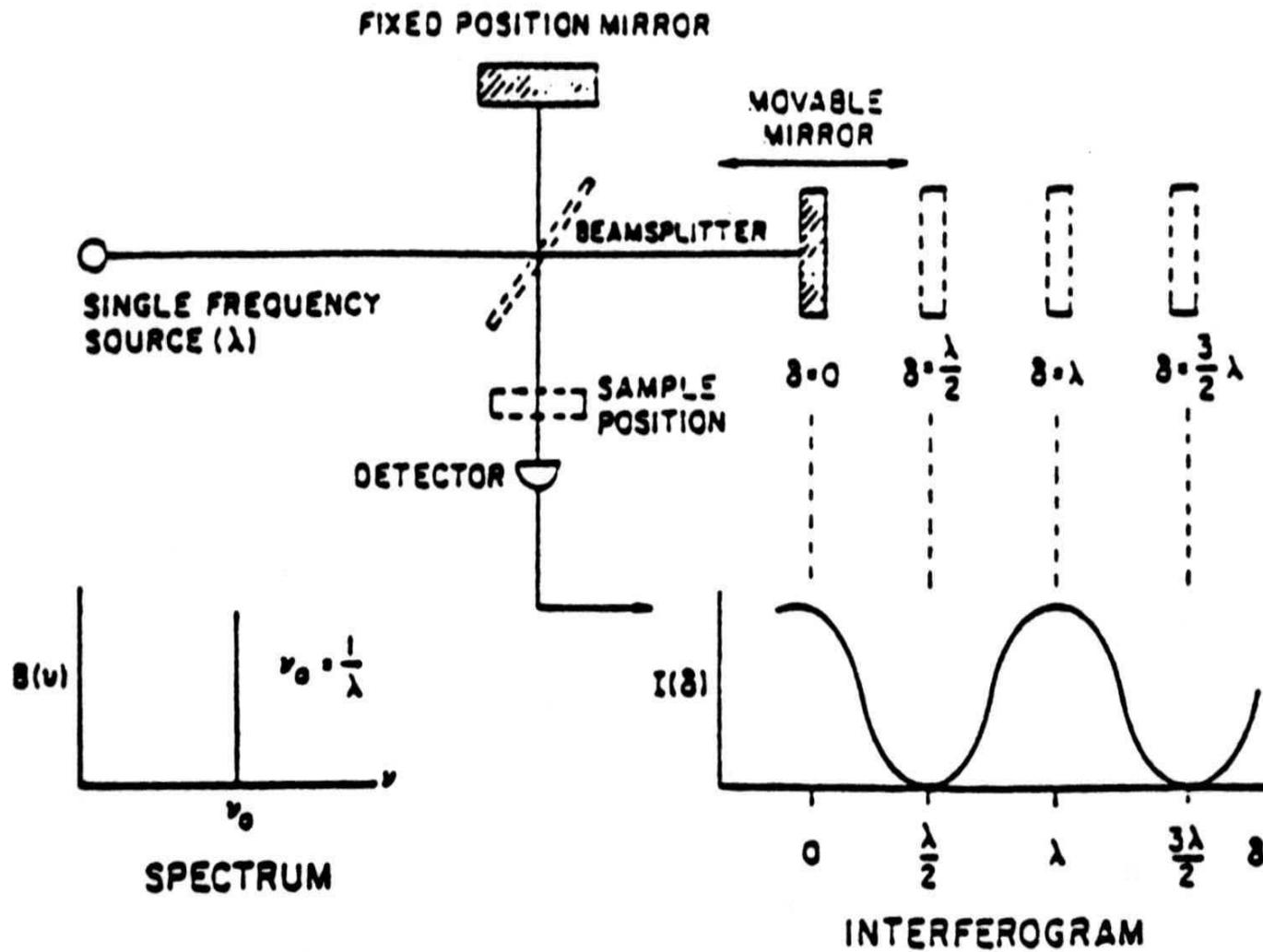
- ▶ Black body radiators
- ▶ Inert solids resistively heated to 1500-2200 K
- ▶ Max radiation between 5000-5900 cm^{-1} (2-1.7 μm), falls off to about 1 % max at 670 cm^{-1} (15 μm)
- ▶ Nernst Glower – cylinder made of rare earth elements
- ▶ Globar- SiC rod
- ▶ CO_2 laser
- ▶ Hg arc (Far IR), Tungsten 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)

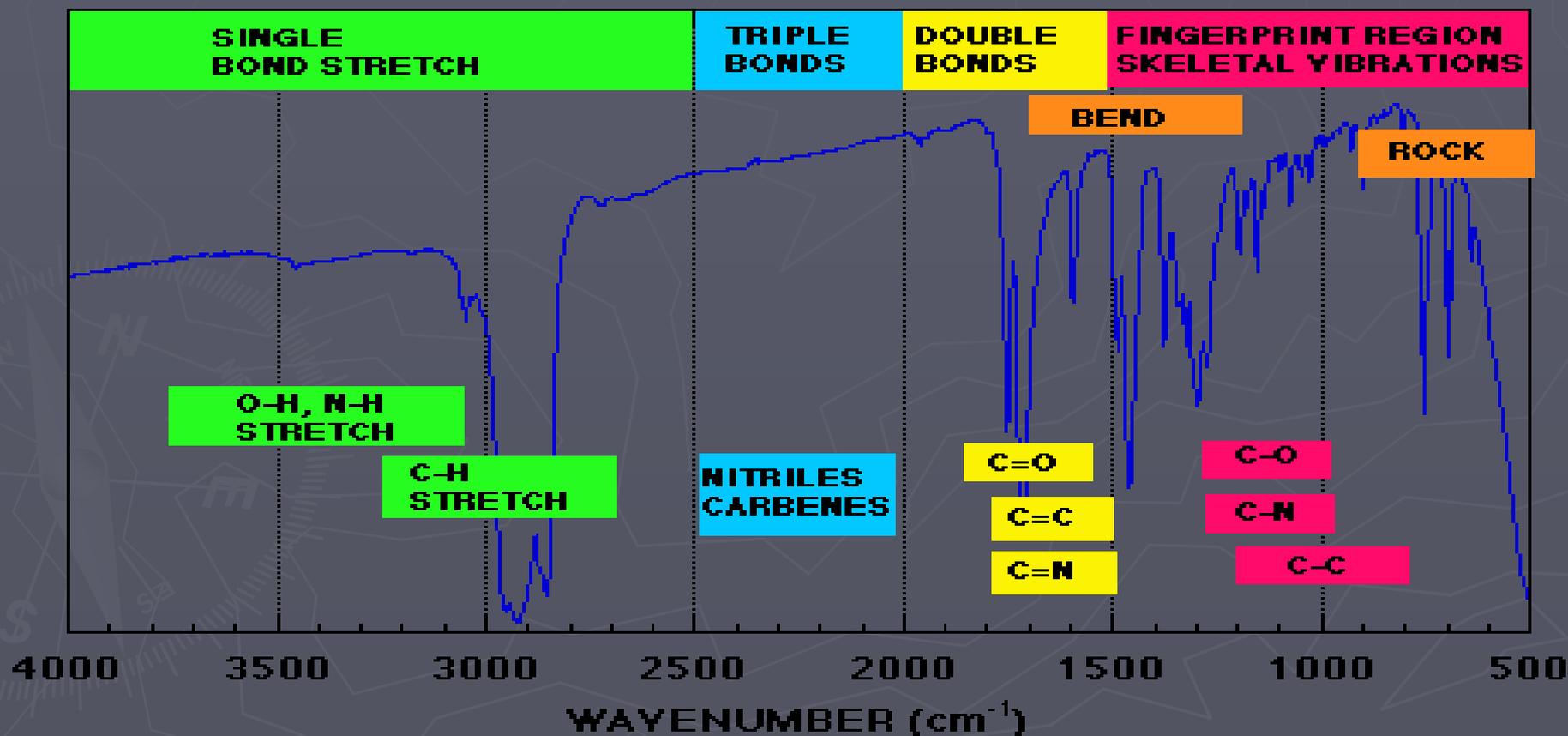
FT-IR detectors

- ▶ 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 cm^{-1} to 1200 cm^{-1}



THANK YOU

