

Infrared Spectroscopy

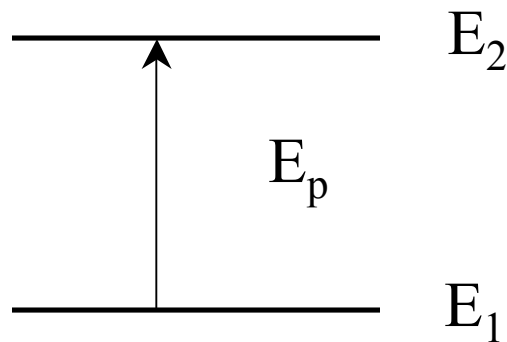
- What is absorption spectroscopy
- What are the physical mechanism of IR absorption
- How is IR spectroscopy used
- Where is FT in FTIR

Absorption Spectroscopy

- EELS
- X-ray absorption spectroscopy
- Atomic absorption spectroscopy (visible or UV light)
- IR spectroscopy

Infrared spectrum

- The wavelength of infrared spectrum is from submicron to hundreds of microns. The region of interest to IR spectroscopy is 1.5-2.5 micron.
- $E_p = E_2 - E_1 = hc/\lambda$ The energy for IR photon is 10^{-3} to 1 eV.



IR Induce Vibration

- For a gas phase molecule

$$E_{\text{Total}} = E_{\text{electronic}} + E_{\text{vibrational}} + E_{\text{rotational}} + E_{\text{translational}}$$

IR can induce vibration, rotation and translation of molecule, but IR spectroscopy only considers the vibration of molecule

Vibration Mode:

1. Stretching mode

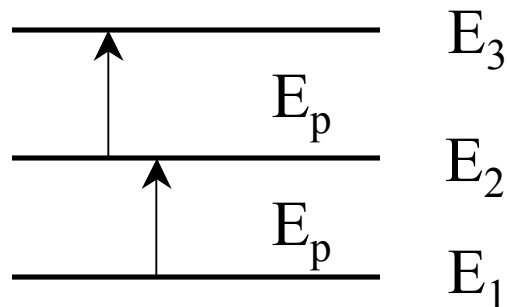
Symmetric or Asymmetric

2. Deformation mode:

scissoring, rocking, wagging, twisting

Interpretation of IR

- Molecular vibrations give rise to IR absorption only if they cause a change in the dipole moment of the molecule.
- No IR absorption for homo-nuclear molecule.
- Highly symmetric molecule exhibit deceptively simple spectrum due to the overlapping (Vibration Degeneration)
- Overtones of fundamental vibration will increase the complexity of IR spectrum



IR Spectra

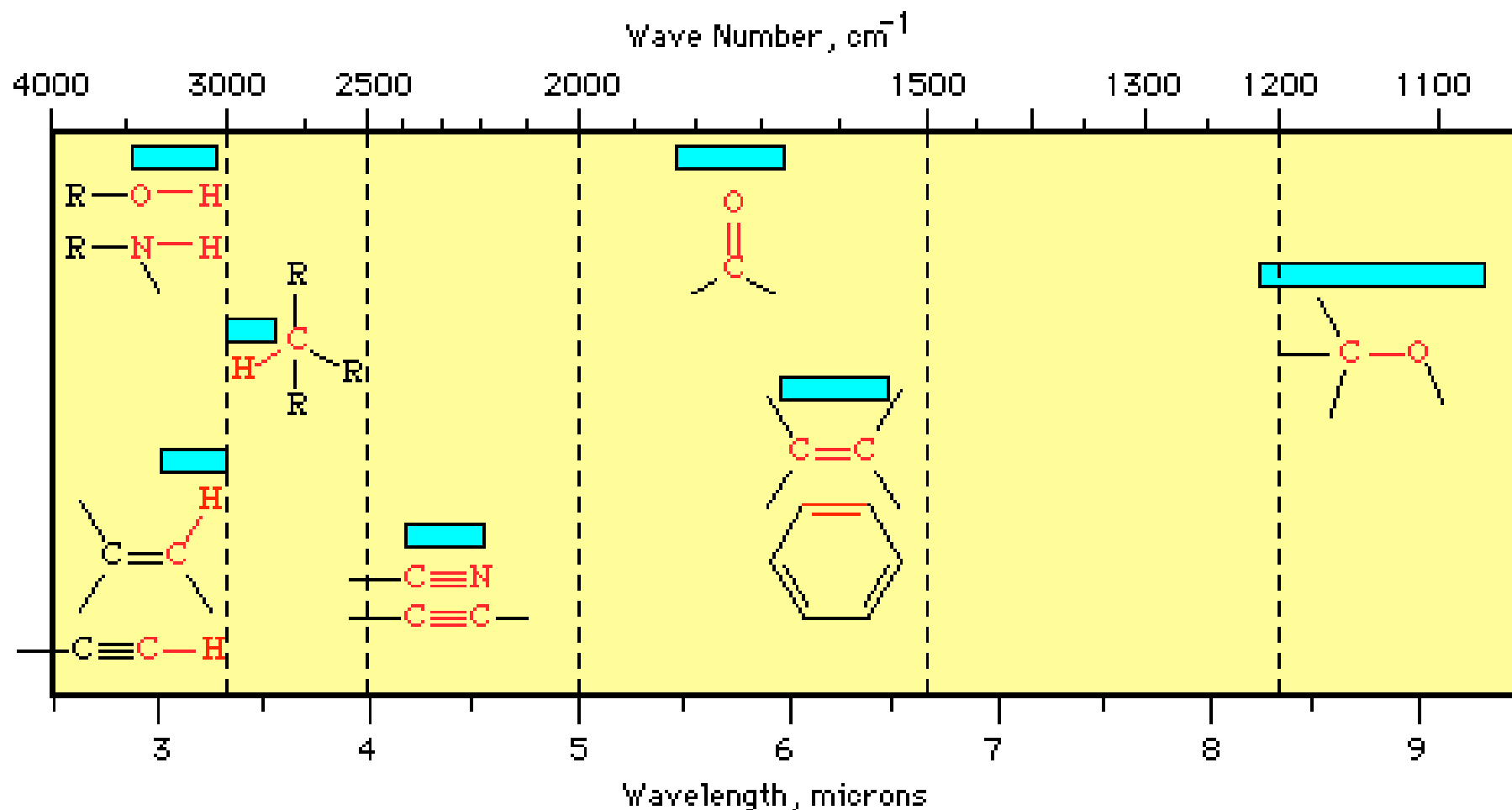
4000-1500 cm^{-1} The Functional Group Region

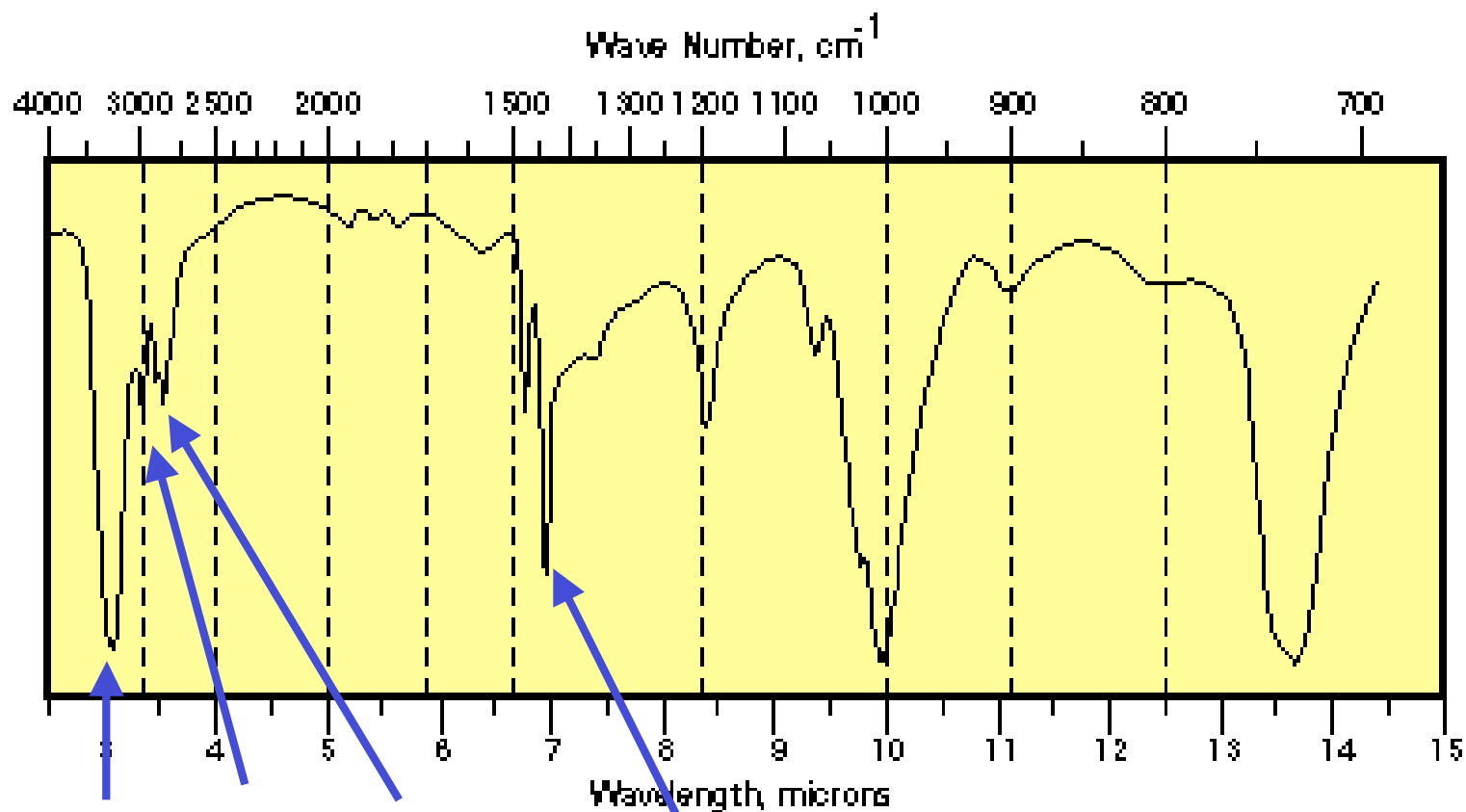
Peaks in this region are characteristic of specific kinds of bonds, and therefore can be used to identify whether a specific functional group is present.

1500-400 cm^{-1} The Fingerprint Region

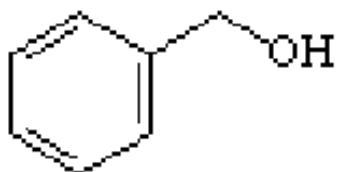
Peaks in this region arise from complex deformations of the molecule. They may be characteristic of molecular symmetry, or combination bands arising from multiple bonds deforming simultaneously.

IR Absorption for Common Groups





-OH C=H C-H

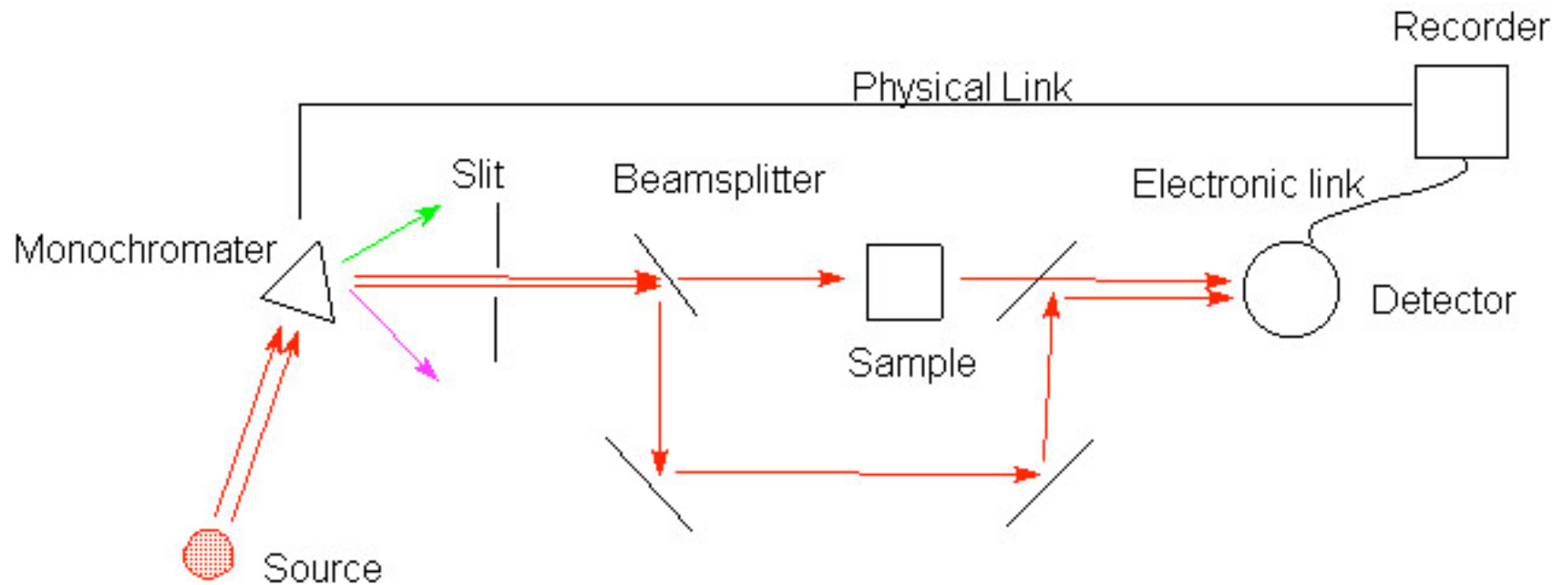


Benzyl Alcohol

Instrumentation

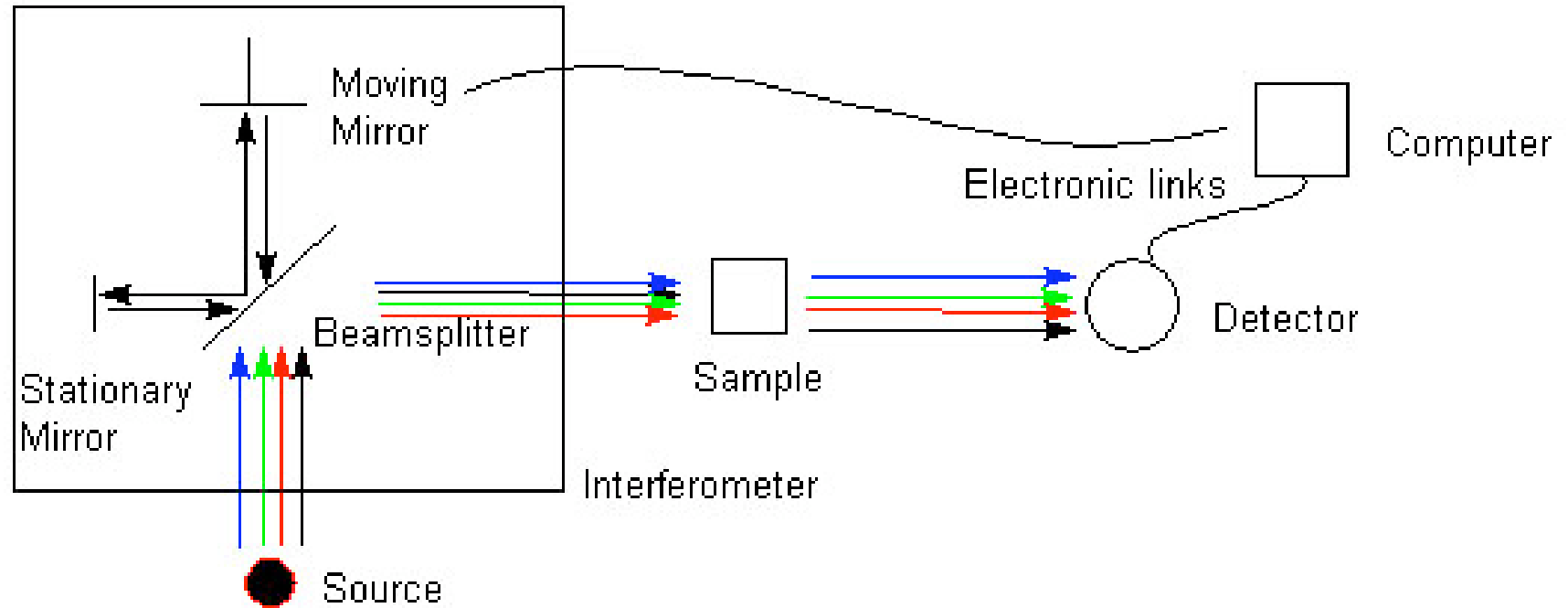
Region	Near IR	Mid-IR	Far-IR
Wavenumber (cm ⁻¹)	12000-4000	4000-200	200-10
Source	W	Nichrome Wire	Hg
Optics	Monochromater	Monochmater /Interferometer	Monochmater /Interferometer
Detector	Pbs photocell	Thermocouple bolometer	Golay cell

Continuous IR



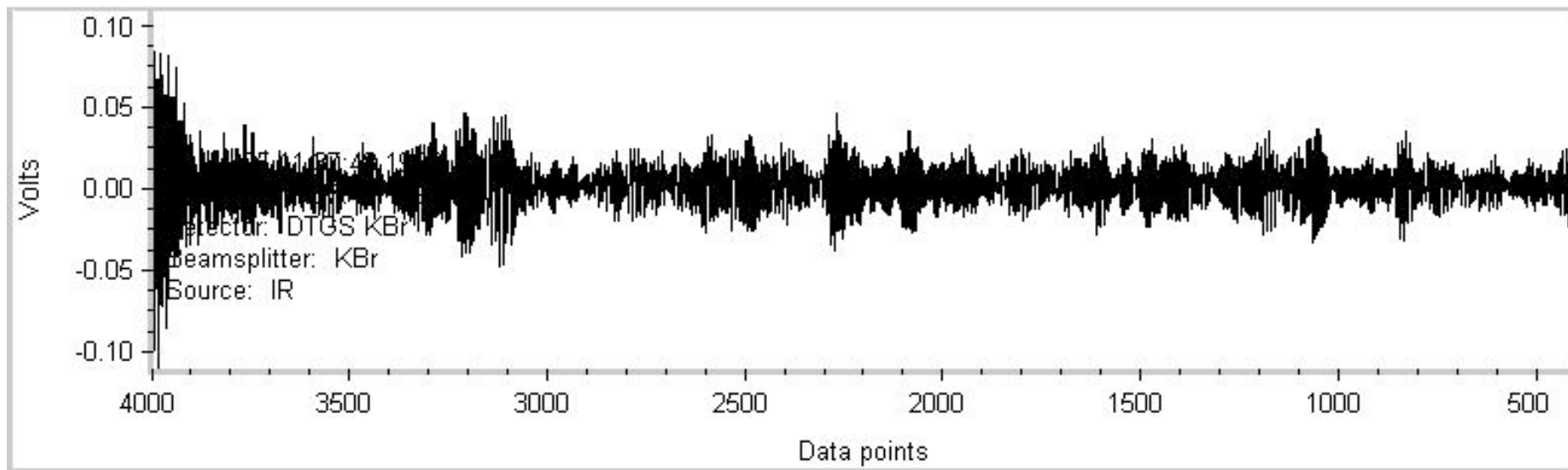
- Monochromator/slit limits the amount of signal for one particular resolution.

FTIR



- All of the source energy gets to the sample, improving the inherent signal-to-noise ratio.
- Resolution is limited by the design of the interferometer (Distance the moving mirror travel)

Interferogram



Spectrum

