Modes of Molecular Vibration Instrumentation of IR and FTIR Spectroscopy

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MOLECULAR VIBRATIONS

The Heisenberg uncertainty principle argues that all atoms in a molecule are constantly in motion (otherwise we would know position and momentum accurately). For molecules, they exhibit three general types of motions: translations (external), rotations (internal) and vibrations (internal). A diatomic molecule contains only a single motion., while polyatomic molecules exhibit more complex vibrations, known as normal modes.

MODES OF MOLECULAR VIBRATIONS

- The normal modes of vibration are:
- Fundamental Vibrations
- Non-Fundamental Vibrations

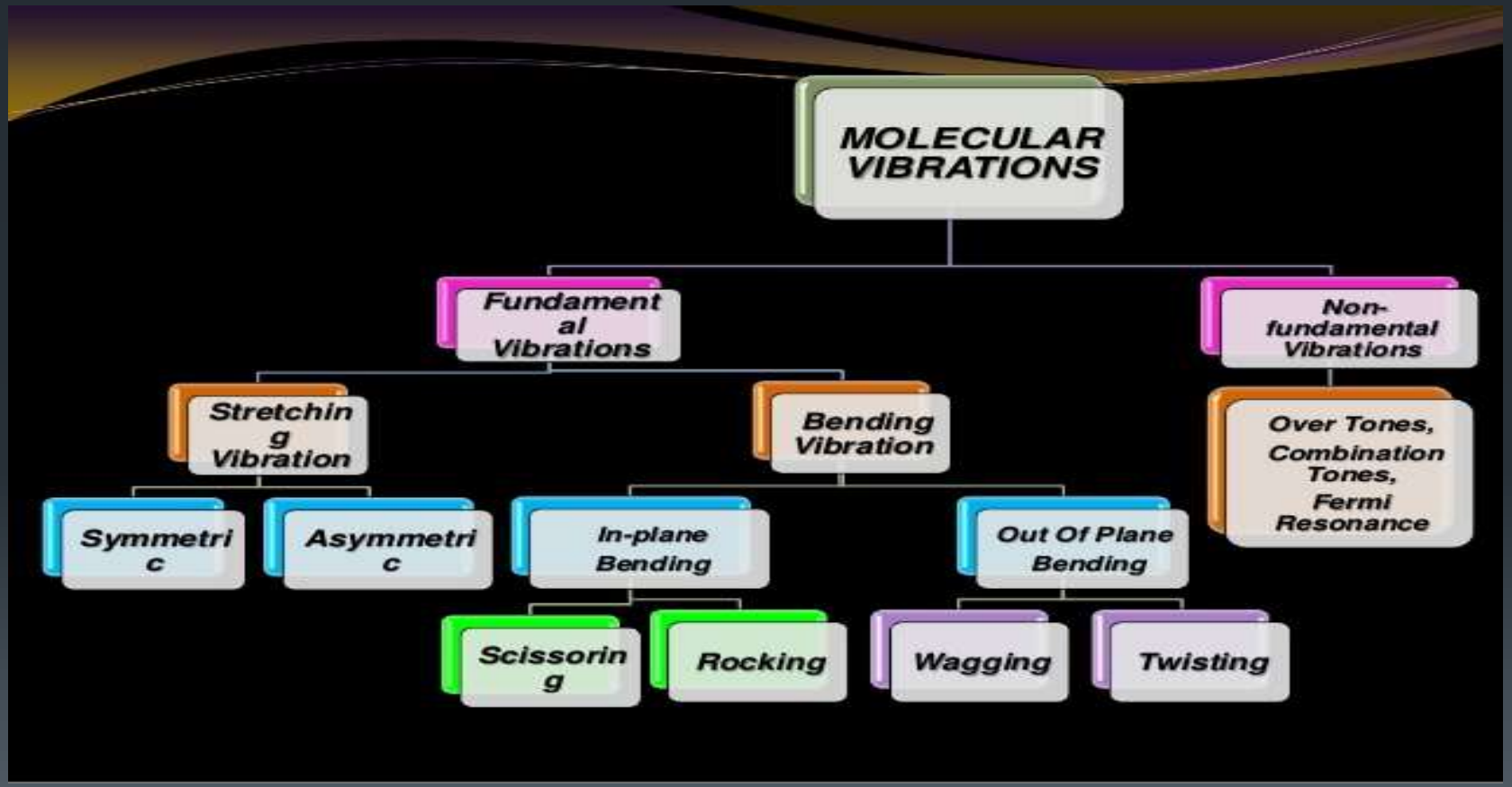
WHAT IS VIBRATION IN MOLECULE?

- ‘Any change in shape of the molecule- streching of bonds, bending of bonds , or internal rotation around single bonds ”.

Why we study the molecular vibration?

- Because whenever the interactions b/w electromagnetic waves & matter occur so change appears in these vibrations

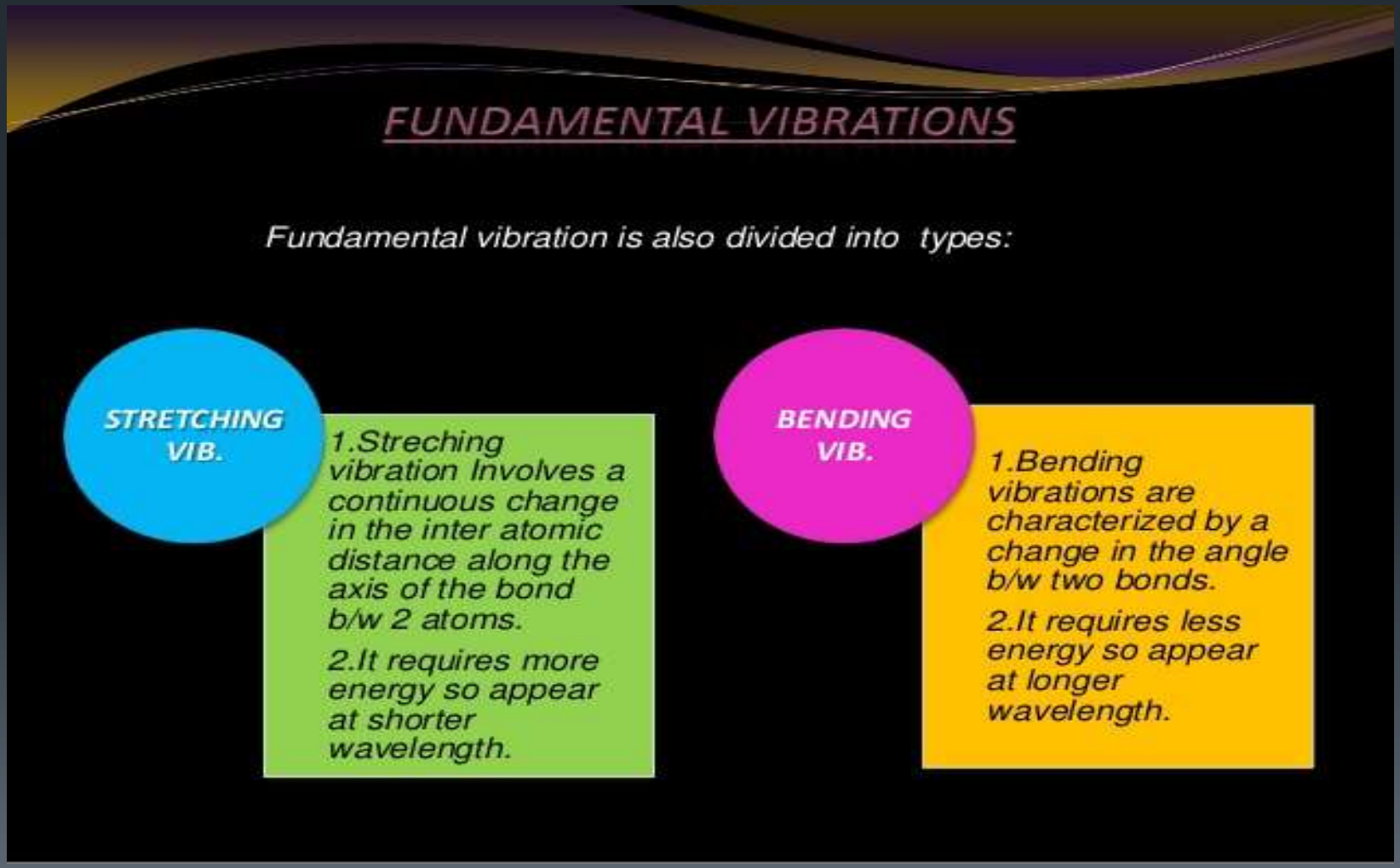
Classification Molecular Vibration



FUNDAMENTAL & NON FUNDAMENTAL VIBRATIONS

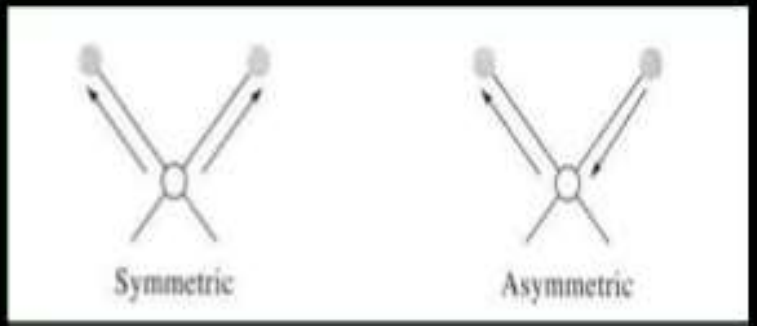
- Vibrations which appears as band in the spectra is known as fundamental vibrations.
- Vibrations which appears as a result of fundamental vibrations is known as non-fundamental .

FUNDAMENTAL VIBRATIONS



Now, streching vibration is further divided into :

SYMMETRIC VIB.	ASYMMETRIC VIB.
• Inter atomic distance b/w 2 atoms increases/decreases.	• Inter atomic distance b/w 2 atoms is alternate/opposite.



Bending vibration is divided into:

IN PLANE BENDING

- *If all the atoms are on same plane.*

OUT OF PLANE BENDING

- *If 2 atoms are on same plane while the 1 atom is on opposite plane.*

In-plane bending further divided into:

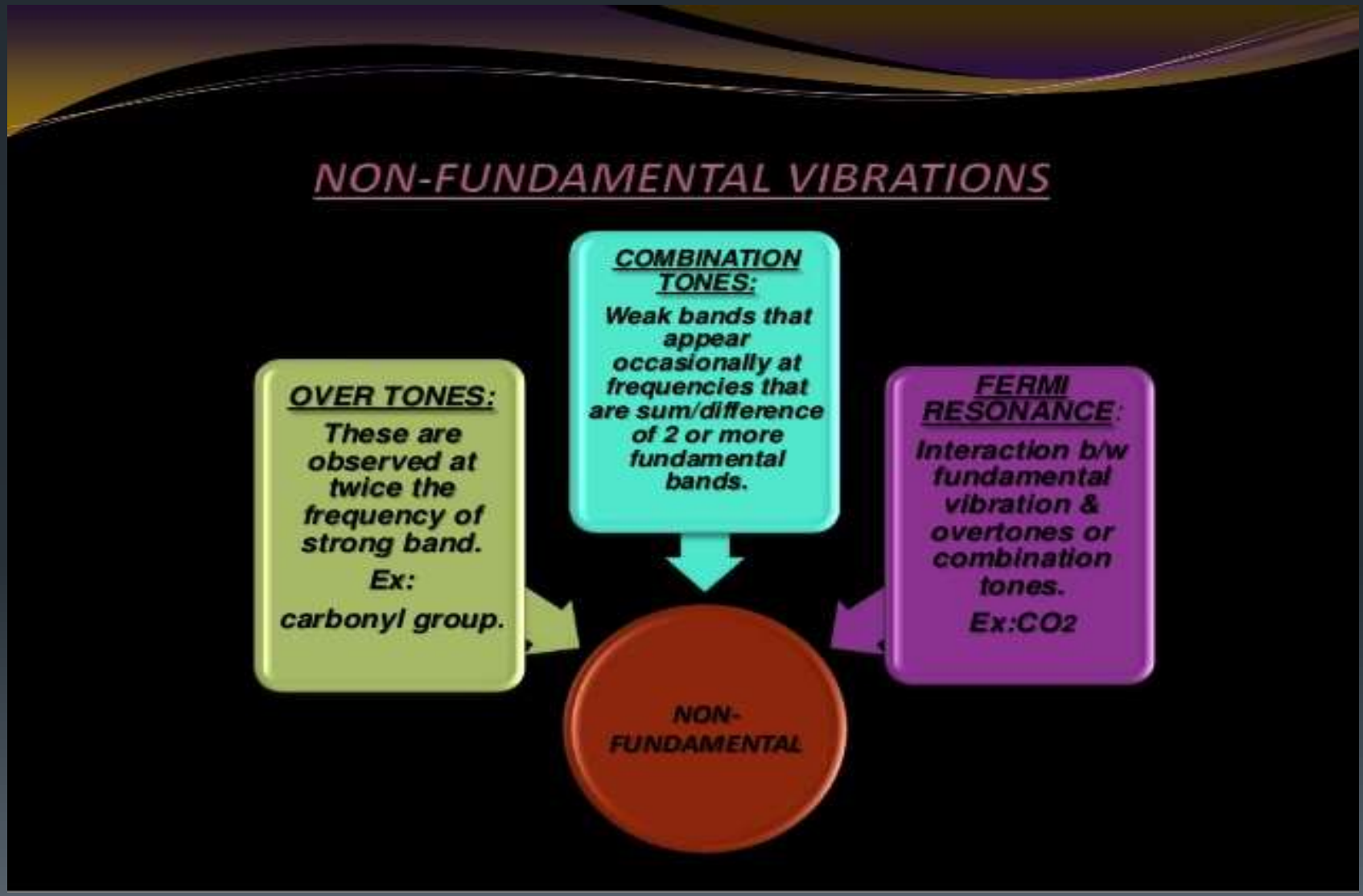
SCISSORING:

When 2 atoms move away or close towards each other.

ROCKING:

Change in angle b/w a group of atoms.

NON-FUNDAMENTAL VIBRATIONS



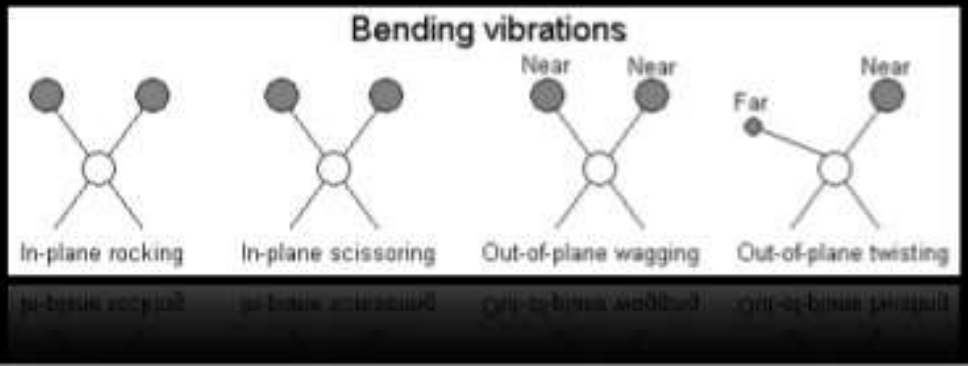
Out plane bending is further divided into:

- Change in angle b/w the plane of a group of atom

WAGGING

TWISTING

- Change in angle b/w the plane of 2 groups of atoms.



DISPERSIVE & FTIR SPECTROMETER

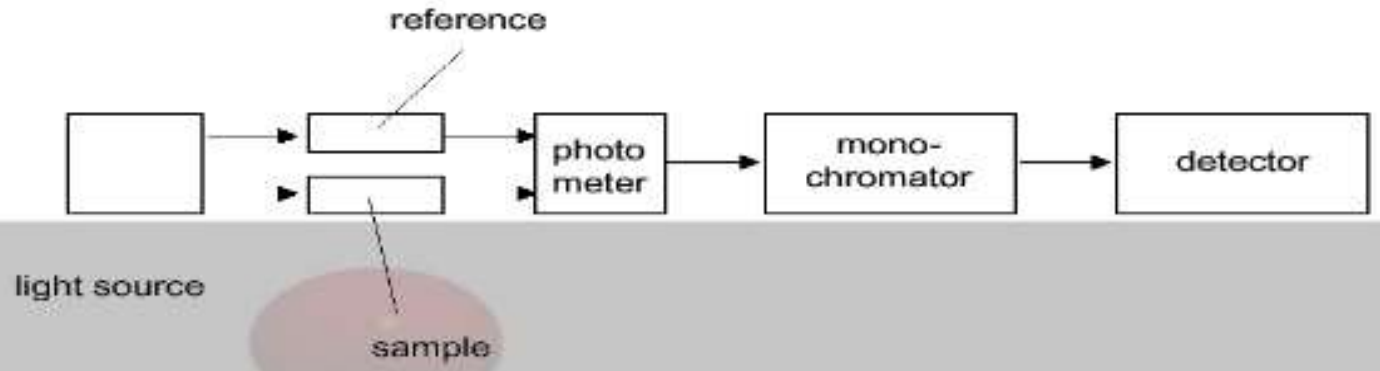
INSTRUMENTATIONS
DISPERSIVE SPECTROMETER

Dispersive IR instruments are introduced in 1940's.

Double-beam instruments are mostly used than Single beam instrument.

In dispersive IR sequential scanning of wave numbers of light takes place.

Instrumentation



In double beam spectrometer , beam separates into two and passes to sample & reference.

Prismatic monochromators have been replaced with Grating monochromator.

Dispersive IR failed due to monochromator containing narrow slits which limit the wave number of radiation.

(X) It containing all movable parts which causes mechanical slippage

(X) Slow scan speed

(X) Less resolution, accuracy and sensitivity

(X) Only narrow frequency range can be studied

(X) Involvement of stray light

(X) Atmospheric absorptions by CO, water also takes place.

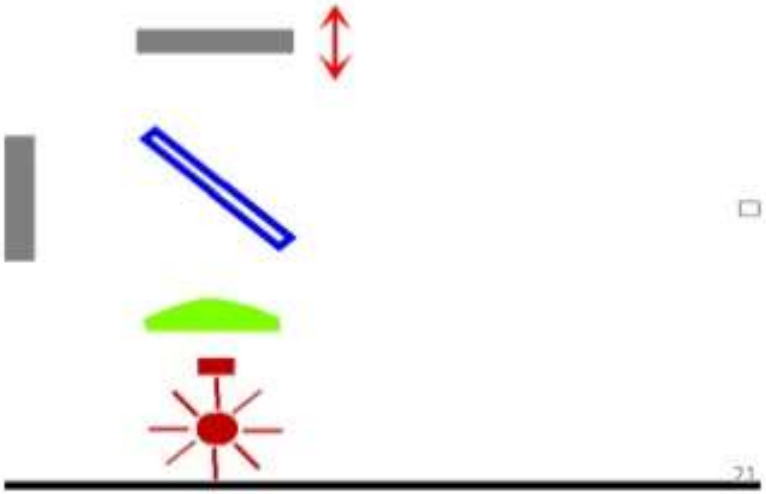
To overcome all these problems FTIR has been developed

Fourier Transform IR Instrument

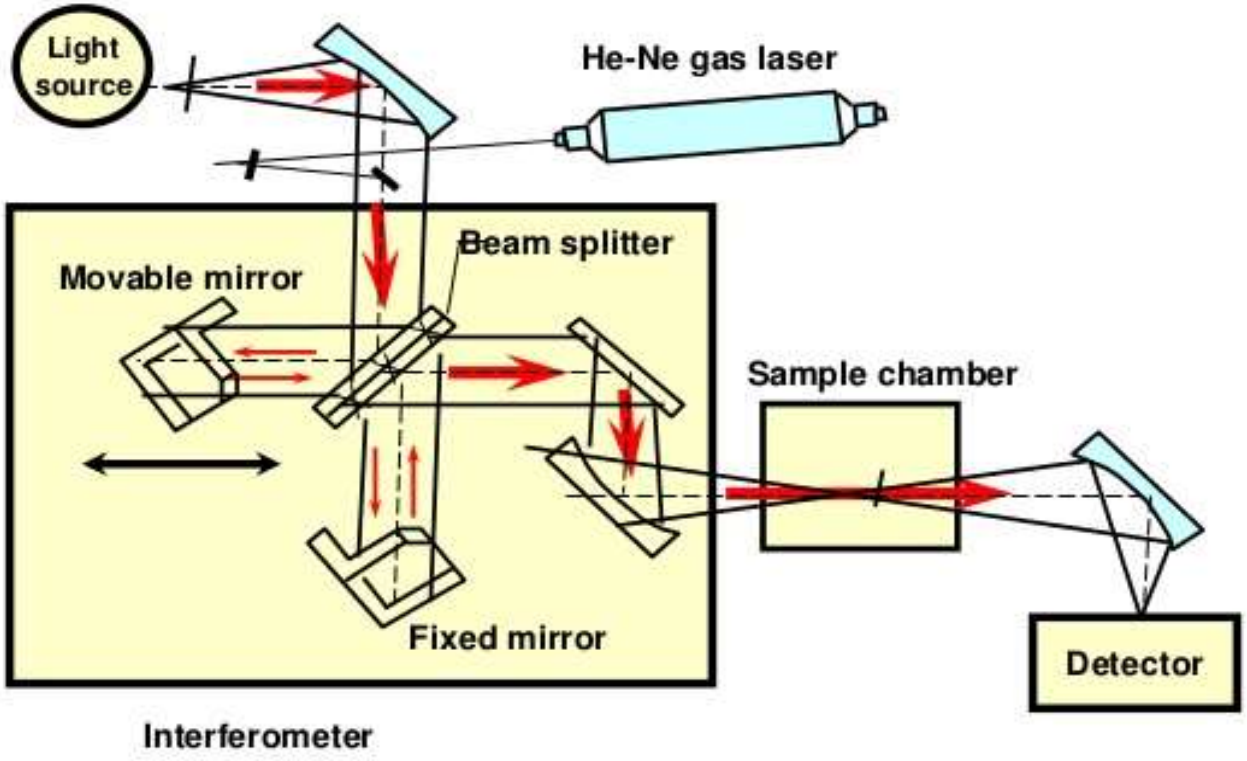
FTIR collects all wavelengths simultaneously and scans at once.

FTIR works based on Michelson Interferometer which having

- Beam splitter
- Fixed mirror
- Movable mirror



FTIR Instrumentation



When the beams are combined an interference pattern is created

Combined beam reaches detector by passing through sample

Obtained spectrum is referred as Interferogram

This will be amplified and translated into IR spectrum by FTIR

Advantages

- ✓ Fast & sensitive
- ✓ All frequencies can be modulated at once
- ✓ Simple mechanical design with only one moving part
- ✓ No stray light is involved
- ✓ When using He-Ne laser as internal standard, no need of external calibration
- ✓ Availability of easy sampling accessories
- ✓ Air pollutants like CO, ethylene oxide etc. can be analysed

Conclusion

FTIR having significant advantages over Dispersive IR due to its fast and accurate analysis.

THANKYOU