IR Spectroscopy

By-
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Introduction :

Gives information about functional groups present in molecule.

- Infrared spectroscopy is the spectroscopy which is concerned with the study of infrared region of electromagnetic spectrum ,which results in vibrational transitions i.e. Study of interaction between infrared radiations & matter.

- It is also called as vibrational spectroscopy.

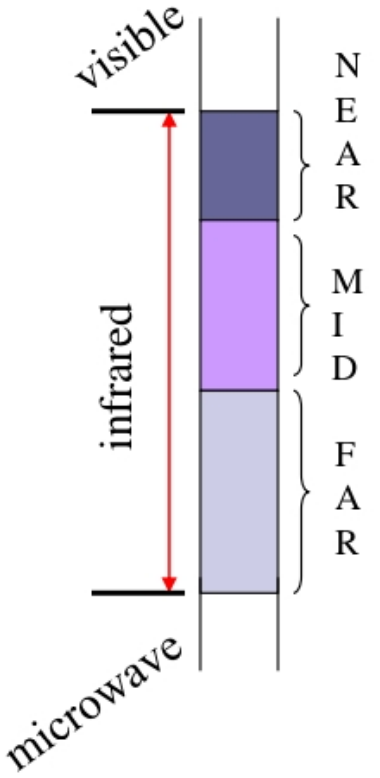
- Vibrations in IR spectroscopy also known as fundamental vibrations.

- It is an important qualitative analytical technique for determining the structure of both organic & inorganic compounds.

- IR region of electromagnetic spectrum:
  - λ : 780 nm – 1000 μm
  - Wavenumber : 12,800 – 10 cm^{-1}

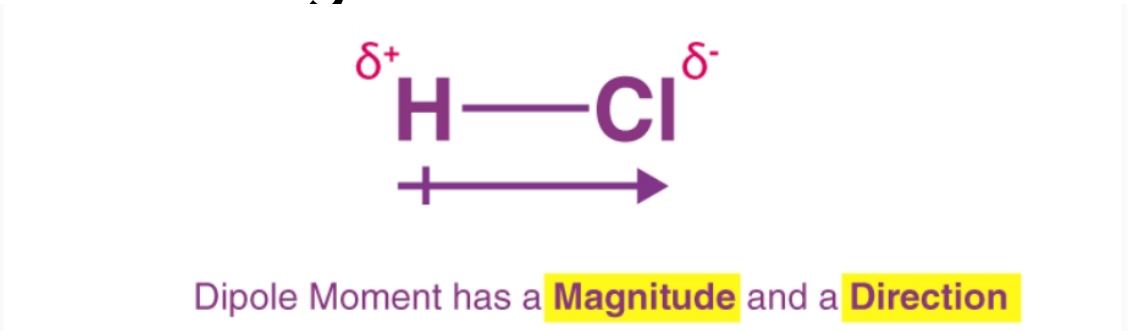
- IR region is subdivided into 3 sub-regions:

1. Near IR region (Nearest to the visible)
   - 780 nm to 2.5 μm (12,800 - 4000 cm^{-1})
2. Mid IR region
   - 2.5 to 50 μm (4000 – 200 cm^{-1})
3. Far IR region
   - 50 to 1000 μm (200 – 10 cm^{-1})



- Molecules are made up of atoms linked by chemical bonds.
- In any molecule, movement of atoms & chemical bond is like spring & balls (vibration).
- This characteristic vibration is called Natural frequency of vibration.
- When energy in the form of infrared radiation is applied then it causes the vibration between the atoms of the molecules & when,
- **Applied infrared frequency= Natural frequency of vibration**

Role of dipole moment in IR spectroscopy :

- The bond dipole moment is a vector quantity since it has both magnitude and direction.
- 

- IR absorption only occurs when IR radiation interacts with a molecule undergoing a change in dipole moment as it vibrates or rotates.
- For a molecule to be IR active there must be a change in dipole moment as a result of the vibration that occurs when IR radiation is absorbed.

Types of vibrations :

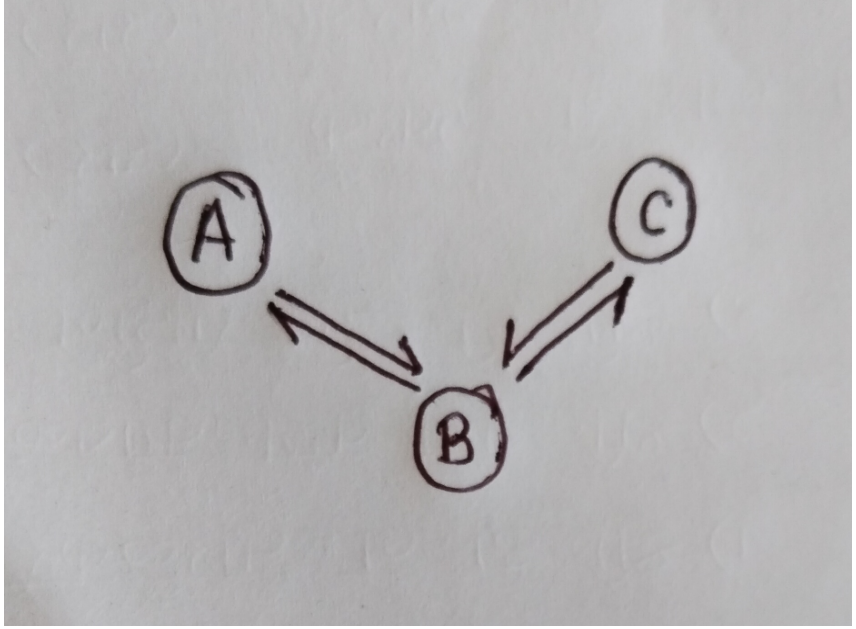
I. **Streching :**

- Bond distance varies.
- Bond angle remains constant.
- 2 types:

① Symetrical streching

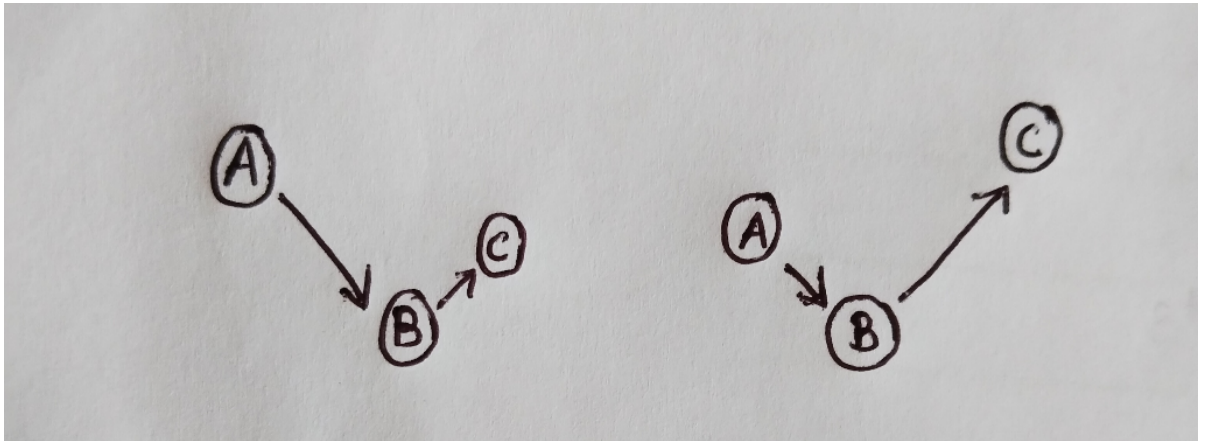
② Asymmetrical streching

1. Symetrical streching :



- In this type of vibration, both **A** & **C** pull away from the **B** and come close to **B** simultaneously.
- If both **A** and **C** are charged, the electrical centre remains unchanged and no change in the dipole moment.
- So the molecules with symmetrical stretching IR inactive.

2. Asymmetrical streching:

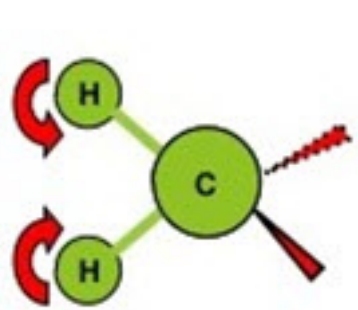


- Here, distance between **A & B** and **B & C** increases or decreases alternatively.
- e.g. When distance between **A** and **B** increases then the distance between **B** and **C** decreases.

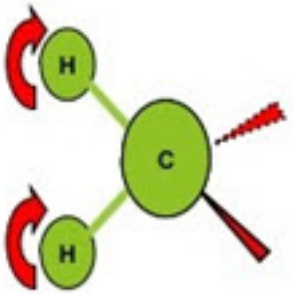
- So the vibrations results into change in dipole moment the molecules are IR active absorbs the radiation.

II. Bending :

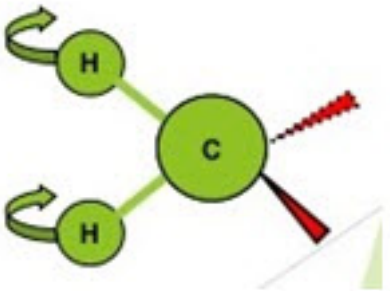
- No change in bonda distance.
- Change in bond angle.



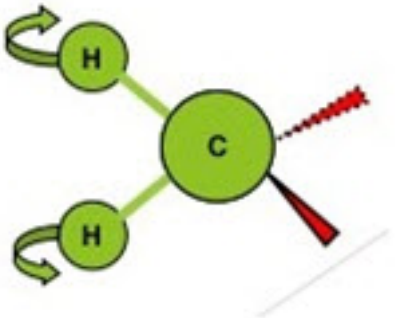
Scissoring



Rocking



Wagging



Twisting

- They involve movement of atoms which are attached to common central atom.
- These are characterized by change in the angle between two bonds.
- Due to bending vibration the shape or confirmation of the molecule is altered which results in change in dipole moment.
- Bending involves less energy and takes place at lower frequencies than stretching.

Principle:

- The principle of IR spectroscopy is related to the vibrational & rotational energy of a molecule.
- When the frequency of the IR radiation is equal to the natural frequency of vibration, the molecule absorb IR radiation
- Absorption of IR radiation causes an excitation of molecule from a lower to the higher vibrational level.

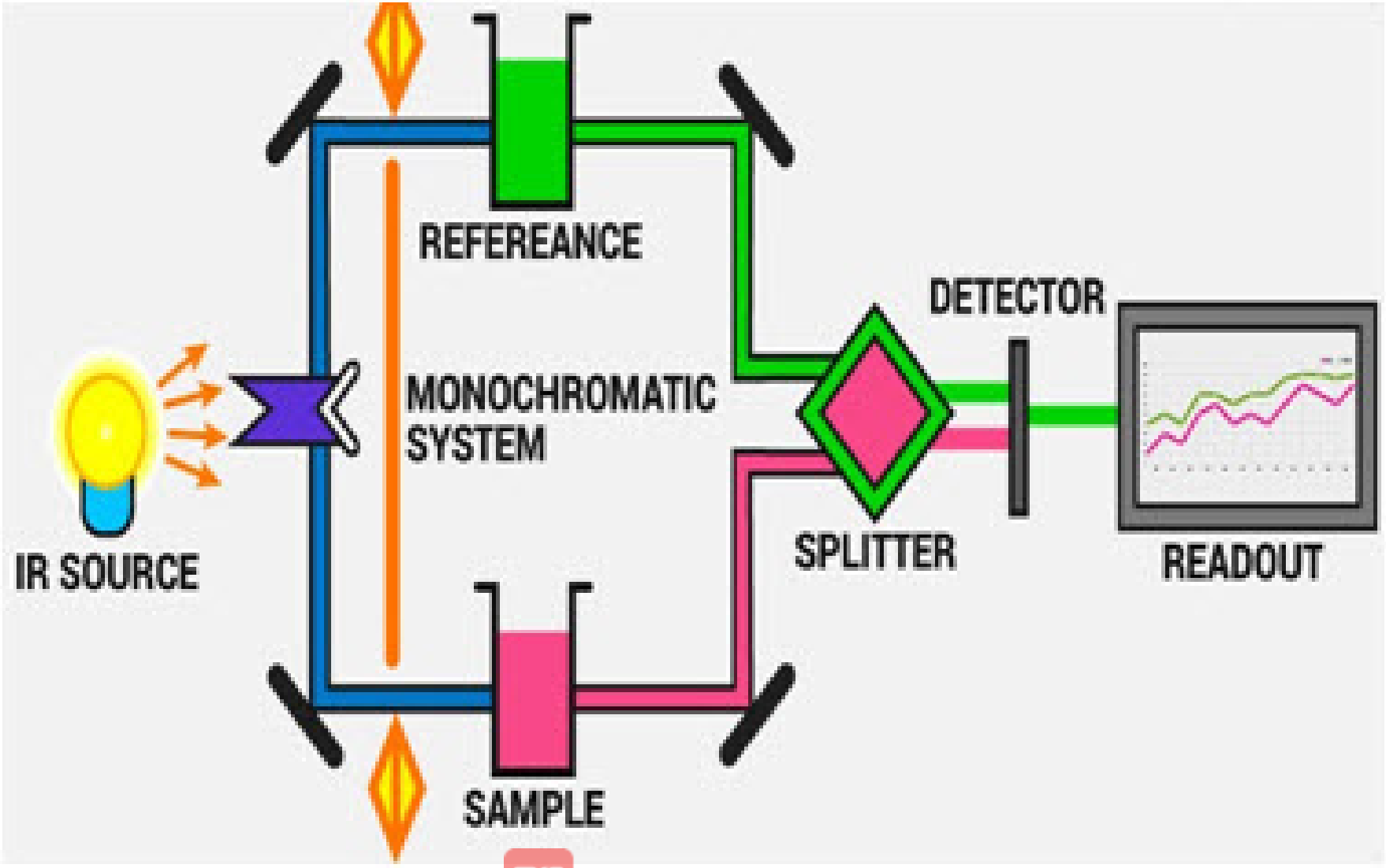
- All the bonds in a molecule are not capable of absorbing IR energy but those bonds which are accompanied by a change in dipole moment will absorb in the IR region & such transitions are called IR active transitions.

- When absorption of IR radiation takes place, a peak is observed.

- Different functional groups absorb characteristic frequencies of IR radiation. Hence gives the characteristic peak value.

- Therefore, IR spectrum of a chemical substance is a finger print of a molecule for its identification.

Instrumentation :



1. Radiation source :

- IR instruments require a source of radiant energy which emits IR radiation which must be steady, intense enough for detection and extend over the desired wavelength.

Near IR region	Tungsten filament
Mid IR region	Nernst glower consists of Zirconium oxide
Far IR region	High pressure mercury lamp

2. Monochromators :

- They convert polychromatic light into monochromatic light

- They must be constructed of materials which transmit IR.

- Two types:

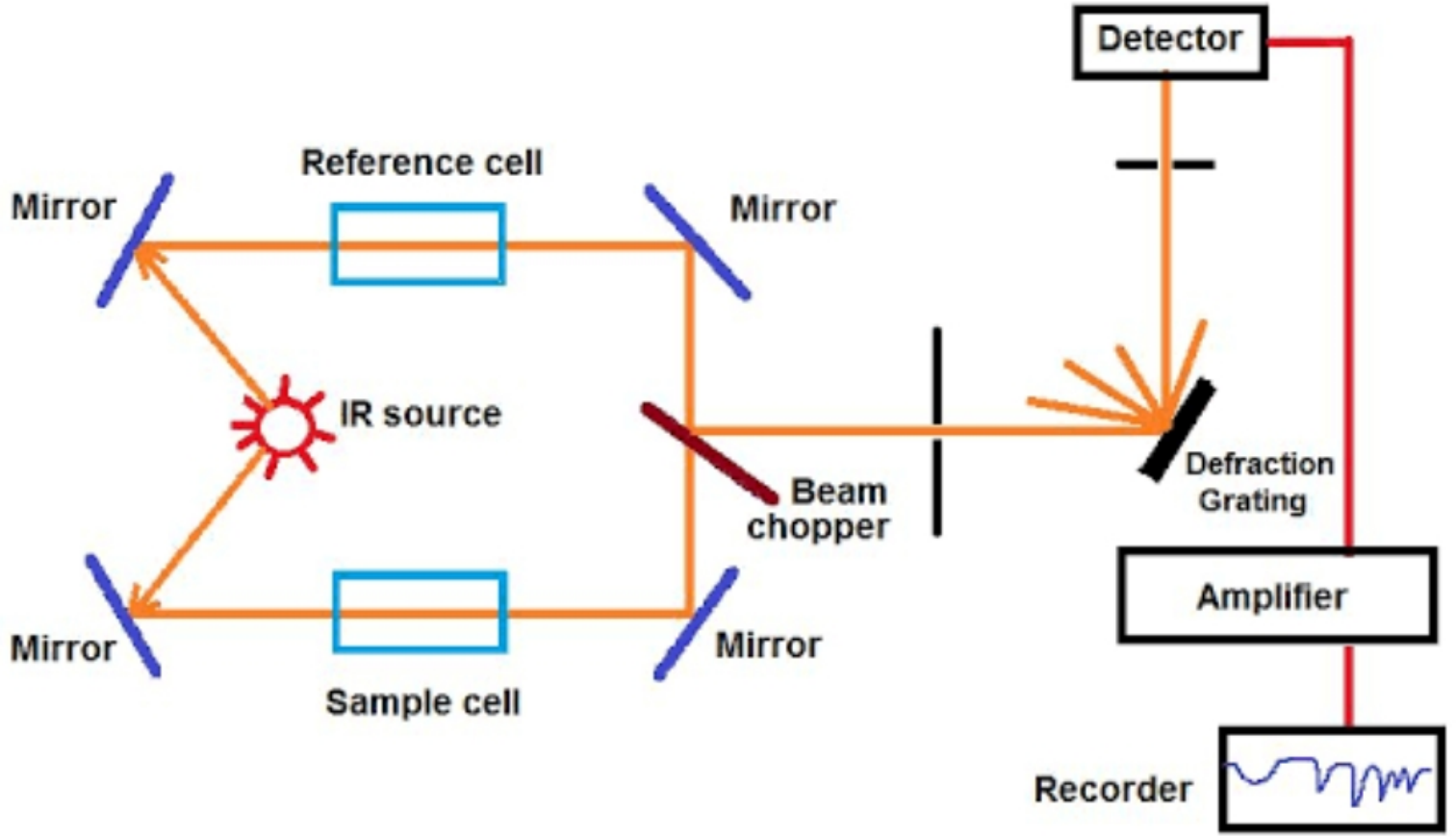
a. Prism monochromator
b. Grating monochromator

- Grating gives better resolution than prism at high temperature.

3.Detector :

- An infrared detector is a detector that reacts to infrared radiation.
- Thermal detectors such as calometer, thermocouples, photoconductivity cell are used.
- The role of detector is to measure unabsorbed IR radiation.

Working :



- Light from the IR source splits into two beams, one of the beam passes through the sample cell ,which is under investigation ,called the **sample beam**, while other beem passes through the reference cell called as a **reference beam**.

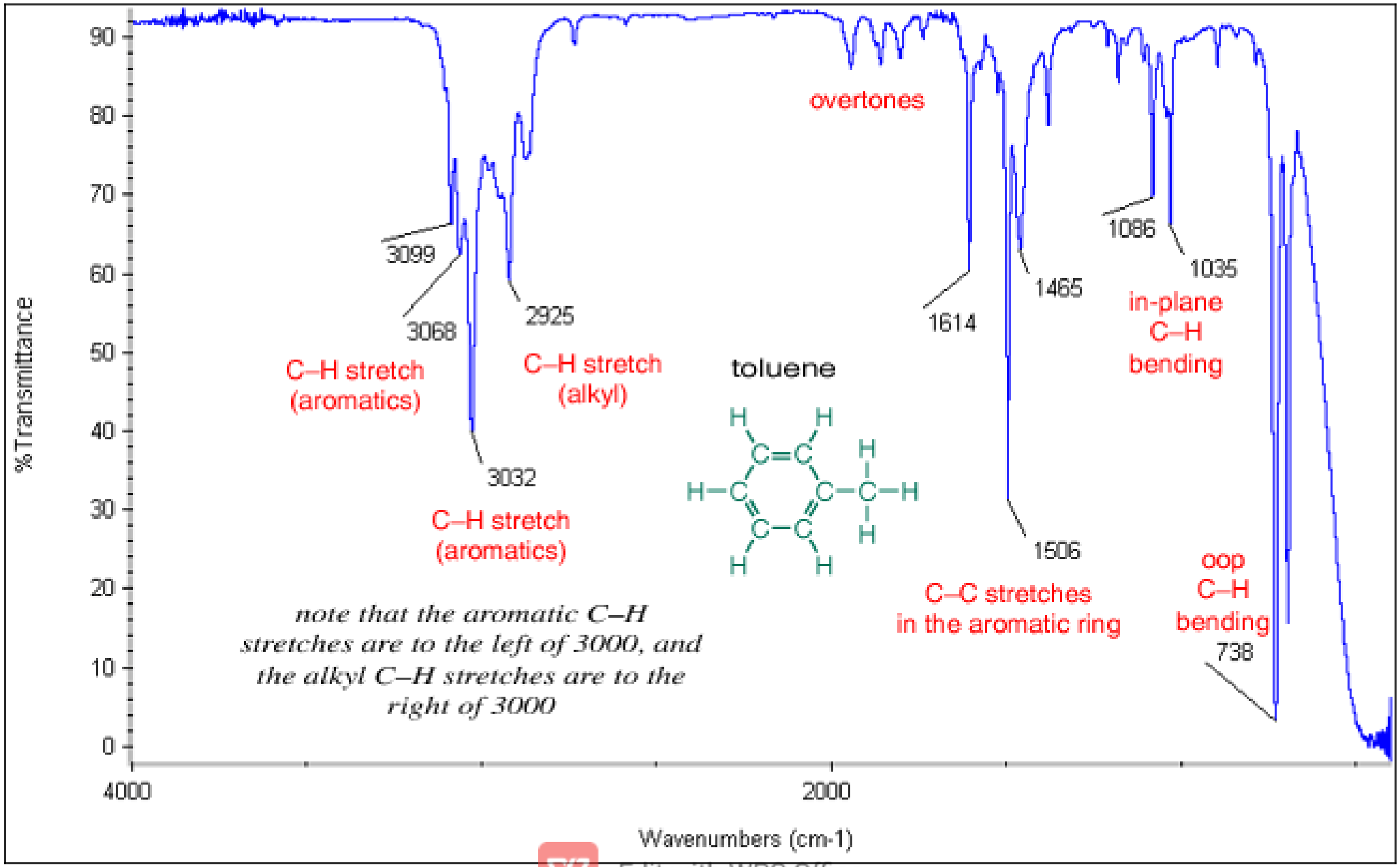
- When the IR beam passes through the sample, its intensity decreases, because some frequencies are absorbed by the sample.

- The detector senses the radiation coming alternatively through the sample and reference cell.

- If the amount of light transmitted is the same in both, it produces direct current and nothing happens.

- But if the intensity of the light coming through the sample and the reference cell are unequal, the detector senses an alternate current which is amplified and recorded.

IR spectrum of Toluene:



Applications :

- Identification of functional group and structure elucidation.
- For characterisation of isolated biological molecules.

Sr. No.	Functional Group	Characteristic Absorption(s) (cm^{-1})
1	Alkyl C-H Stretch	2950 - 2850 (m or s)
2	Alkenyl C-H Stretch Alkenyl C=C Stretch	3100 - 3010 (m) 1680 - 1620 (v)
3	Alkynyl C-H Stretch Alkynyl C≡C Stretch	~3300 (s) 2260 - 2100 (v)
4	Aromatic C-H Stretch Aromatic C-H Bending Aromatic C=C Bending	~3030 (v) 860 - 680 (s) 1700 - 1500 (m,m)
5	Alcohol/Phenol O-H Stretch	3550 - 3200 (broad, s)
6	Carboxylic Acid O-H Stretch	3000 - 2500 (broad, v)
7	Amine N-H Stretch	3500 - 3300 (m)
8	Nitrile C≡N Stretch	2260 - 2220 (m)
9	Aldehyde C=O Stretch Ketone C=O Stretch Ester C=O Stretch Carboxylic Acid C=O Stretch Amide C=O Stretch	1740 - 1690 (s) 1750 - 1680 (s) 1750 - 1735 (s) 1780 - 1710 (s) 1690 - 1630 (s)
10	Amide N-H Stretch	3700 - 3500 (m)

- **Identification of substances:**

IR spectroscopy is used to establish whether a given sample of an organic substance is identical with another or not.

- **Pharmaceutical applications:**

To study the ingredients of drug formulation.

- **Study of microbial cell spectra :**

due to presence of proteins and nucleic acid.