FTIR

Infrared spectroscopy

Infrared spectroscopy is concerned with the absorption of infrared radiation, which results in vibrational transitions. IR spectra are mainly used in structure detection to determine the functional groups. It is already known that,

Energy of a molecule= Electronic energy + Vibrational energy + Rotational energy

Principle:

In any molecule, it is known that atoms or groups of atoms are connected by different types of bonds. These are analogous to springs and non-rigid in by virtue. Because of the continuous motion of the molecule, they express some vibrations with a specific frequency, characteristics to throughout the molecule which is known as Natural frequency of vibration.

Applied infrared frequency = Natural frequency of vibration,

As the IR radiation takes place by absorbing a particular spectrum, a peak is observed. Every bond and its pattern of molecule or functional group require a specific frequency for absorption. Hence every functional group or part of the molecule shows characteristic peak. In other words, IR spectra can be bitterly defined as finger print of a molecule. In pharmaceutical analysis, the range of infrared radiation (mid-IR) we used at a wavelength 25µ to 2.5µ or wave numbers from 400cm-1 to 4000cm-1 There are other region like near –IR (0.8mg to 2.5 mg) and far –IR (25-1000mg) which are not used in pharmacy. Generally, we use wave numbers in IR spectra instead of wave lengths for mentioning the characteristic peak, because wave numbers are larger values as well as easy to handle. On the other side, the wavelengths show a little difference between functional groups.

Wave number can be defined as the number of waves present per cm, which can be calculated from the wavelength.

1/wavelength in μ *104 = wave number per cm or cm-1

Group frequency region- 4000cm- to 1500cm-1

Finger print region- 1500cm-1 to 400cm-1

Criteria for a compound to absorb IR radiation

1. Change or modify in dipole moment

2. Applied IR frequency should be equal to the natural frequency of radiation.

Table- 60: Standard list of Particals group and its ranges (cm^{-1}).

Group	Range (cm^{-1})
C-H stretching (alkane)	2960-2850
C-H stretching(alkene)	3040-3010
C-H stretching(aromatic)	3030
C-H bending (alkane)	1340
C-H bending(aromatic)	700-850
C=C stretching (alkene)	1680-1620
C=C stretching (alkyne)	2100-2200
C=C stretching (aromatic)	1450-1600
C=O stretching (ketone)	1705-1725
C=O stretching (aldehyde)	1720-1740
C=O stretching (ester)	1735-1750
C=O stretching (acid)	1700-1725
C=O stretching(amide)	1650-1700
O-H stretching (Free)	3590-3650
O-H stretching(alcohols)	1050-1150
O-H bending (phenols)	1200
O-H bending (alcohols)	1250-1350
C-O stretching (phenols)	1310-1410
N- H stretching	3400-3500
N-H bending	1500-1650
C-N vibrations	1000-1400
C=N stretching	2240-2260
C=N stretching	1630-1690
N=N stretching	1575-1630
S-H stretching	2500-2600
C=S stretching	1050-1200
S=O stretching	1050-1400