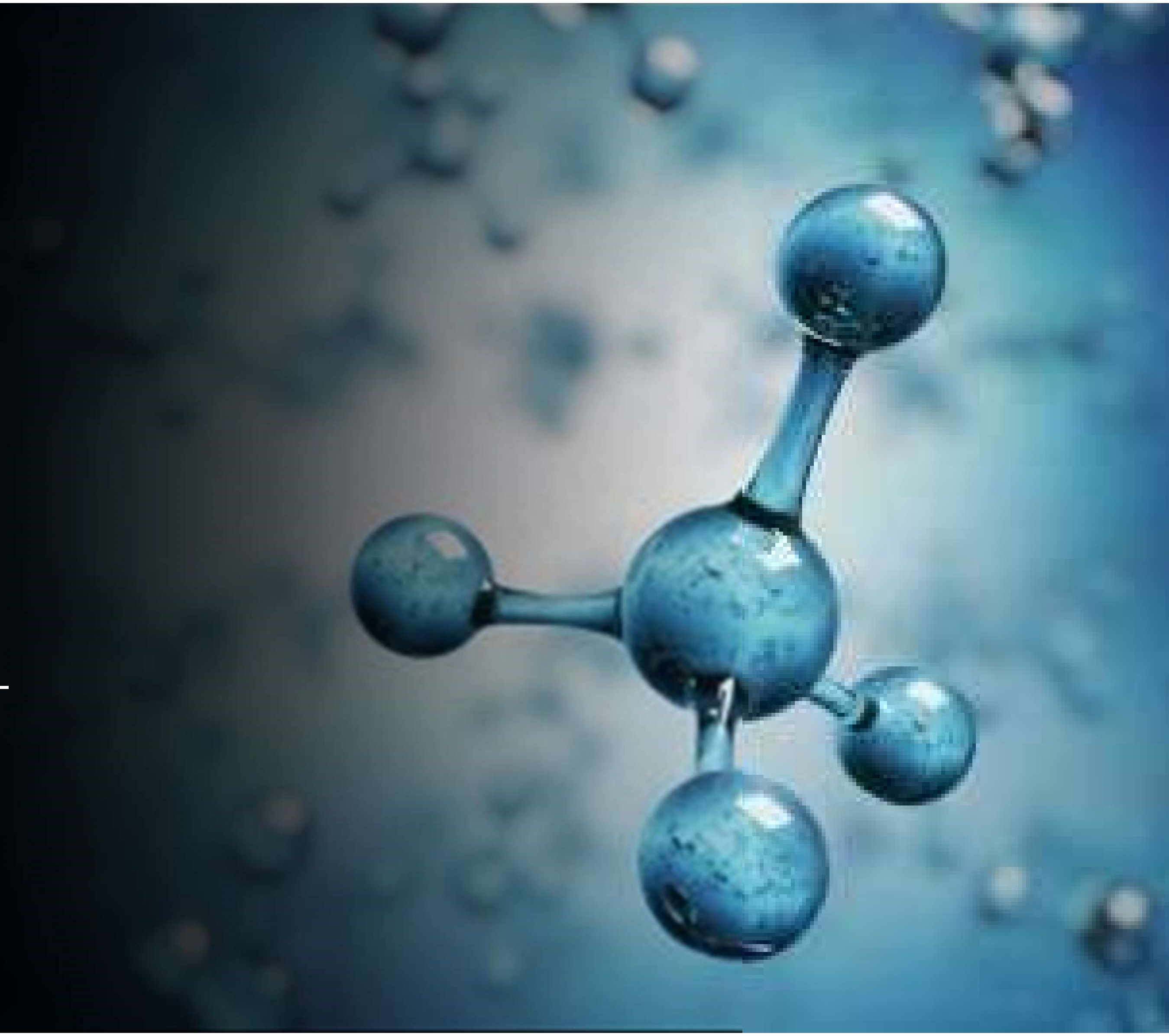
IR spectroscopy



- Spectroscopy is a technique used to determine the structure of a compound by the study of the interaction between **matter** and **electromagnetic radiation**

- Nondestructive (destroys little or no sample).

EMR → ANALYTE → SPECTROPHOTOGRAPH

1.UV-Visible radiations--------excitation of electrons---------UV-visible spectrum

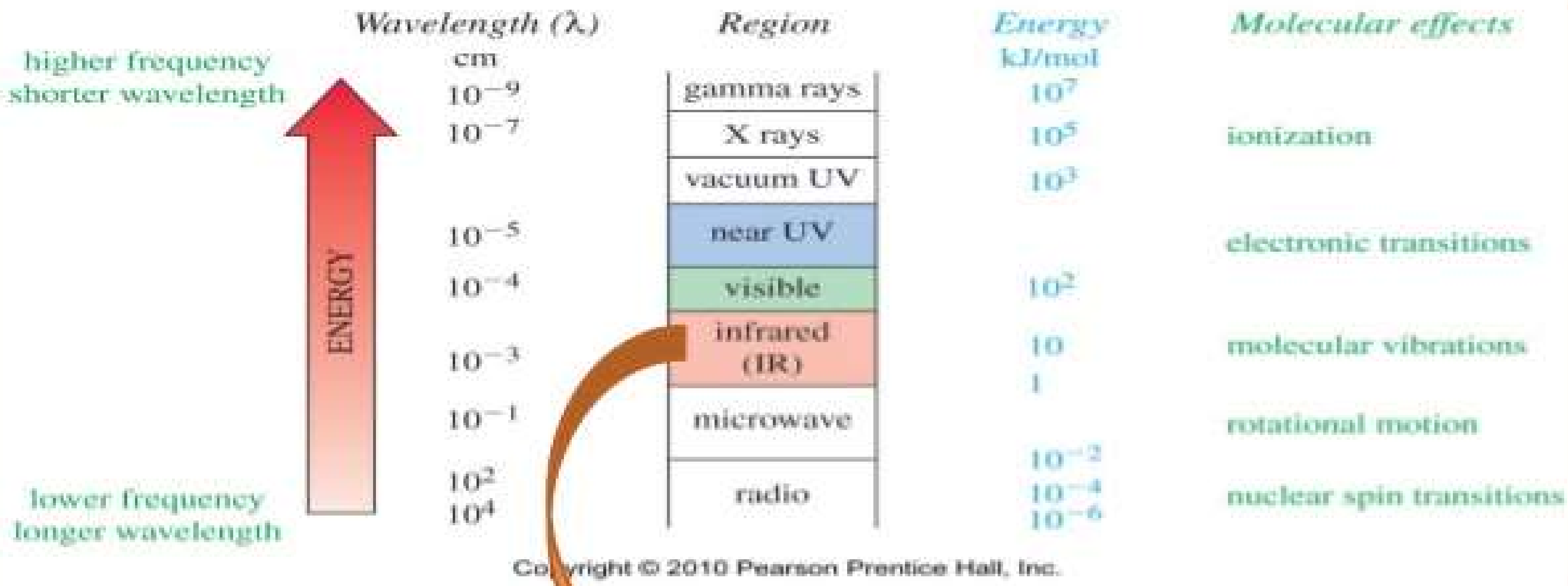
2.IR-radiations----------------------vibration changes -------------------IR spectrum

3.Radio frequency--------------spin rotational changes------------N.M.R spectrum

TYPES OF SPECTROSCOPY

- UV- Vis spectroscopy uses electronic transitions to determine bonding patterns
- Infrared (IR) spectroscopy measures the bond vibration frequencies in a molecule and is used to determine the functional group.
- Nuclear magnetic resonance (NMR) spectroscopy analyzes the environment of the hydrogens in a compound. This gives useful clues as to the alkyl and other functional groups present.
- Mass spectrometry (MS) fragments the molecule and measures their mass. MS can give the molecular weight of the compound and functional groups

THE ELECTROMAGNETIC SPECTRUM

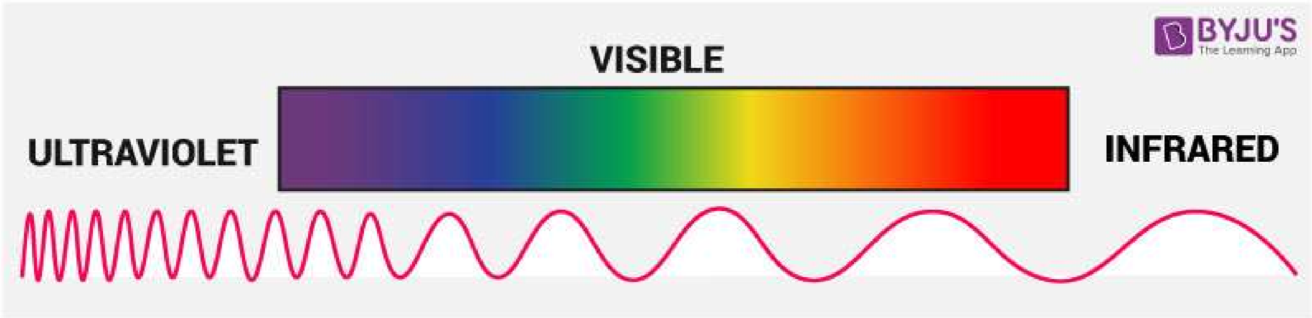


IR REGIONS	RANGE
Near infrared region	*0.8-2.5 μ (12,500 - 4000 cm-1)*
Mid infrared region	*2.5-15 μ (4000 - 667cm-1)*
Far infrared region	*15-200 μ (667 - 50 cm-1)*

IR spectroscopy

- IR spectroscopy (which is short for infrared spectroscopy) deals with the infrared region of the electromagnetic spectrum, i.e. light having a longer wavelength and a lower frequency than visible light. Infrared Spectroscopy generally refers to the analysis of the interaction of a molecule with infrared light.
- The IR spectroscopy concept can generally be analyzed in three ways: by measuring reflection, emission, and absorption. The major use of infrared spectroscopy is to determine the functional groups of molecules, relevant to both organic and inorganic chemistry

An IR spectrum is essentially a graph plotted with the infrared light absorbed on the Y-axis against. frequency or wavelength on the X-axis. An illustration highlighting the different regions that light can be classified into is given below.
IR Spectroscopy detects frequencies of infrared light that are absorbed by a molecule. Molecules tend to absorb these specific frequencies of light since they correspond to the frequency of the vibration of bonds in the molecule.



The energy required to excite the bonds belonging to a molecule, and to make them vibrate with more amplitude, occurs in the Infrared region. A bond will only interact with the electromagnetic infrared radiation, however, if it is polar.

The presence of separate areas of partial positive and negative charge in a molecule allows the electric field component of the electromagnetic wave to excite the vibrational energy of the molecule.

The change in the vibrational energy leads to another corresponding change in the dipole moment of the given molecule. The intensity of the absorption depends on the polarity of the bond. Symmetrical non-polar bonds in N≡N and O=O do not absorb radiation, as they cannot interact with an electric field.

Regions of the Infrared spectrum

Most of the bands that indicate what functional group is present are found in the region from 4000 cm-1 to 1300 cm-1. Their bands can be identified and used to determine the functional group of an unknown compound.

Bands that are unique to each molecule, similar to a fingerprint, are found in the fingerprint region, from 1300 cm-1 to 400 cm-1. These bands are only used to compare the spectra of one compound to another.

Samples in Infrared Spectroscopy

The samples used in IR spectroscopy can be either in the solid, liquid, or gaseous state.

- Solid samples can be prepared by crushing the sample with a mulling agent which has an oily texture. A thin layer of this mull can now be applied on a salt plate to be measured.
- Liquid samples are generally kept between two salt plates and measured since the plates are transparent to IR light. Salt plates can be made up of sodium chloride, calcium fluoride, or even potassium bromide.
- Since the concentration of gaseous samples can be in parts per million, the sample cell must have a relatively long pathlength, i.e. light must travel for a relatively long distance in the sample cell.

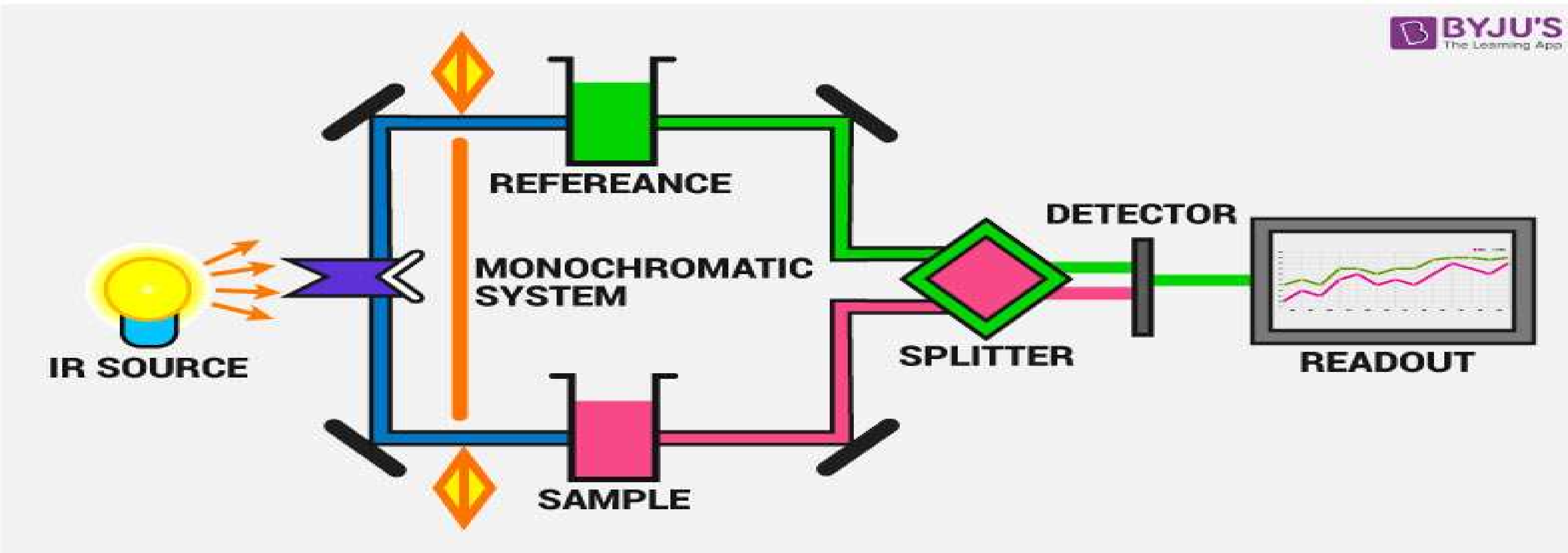
Thus, samples of multiple physical states can be used in Infrared Spectroscopy.

Principle Of Infrared Spectroscopy

- The IR spectroscopy theory utilizes the concept that molecules tend to absorb specific frequencies of light that are characteristic of the corresponding structure of the molecules. The energies are reliant on the shape of the molecular surfaces, the associated vibronic coupling, and the mass corresponding to the atoms.
- For instance, the molecule can absorb the energy contained in the incident light and the result is a faster rotation or a more pronounced vibration.

IR Spectroscopy Instrumentation

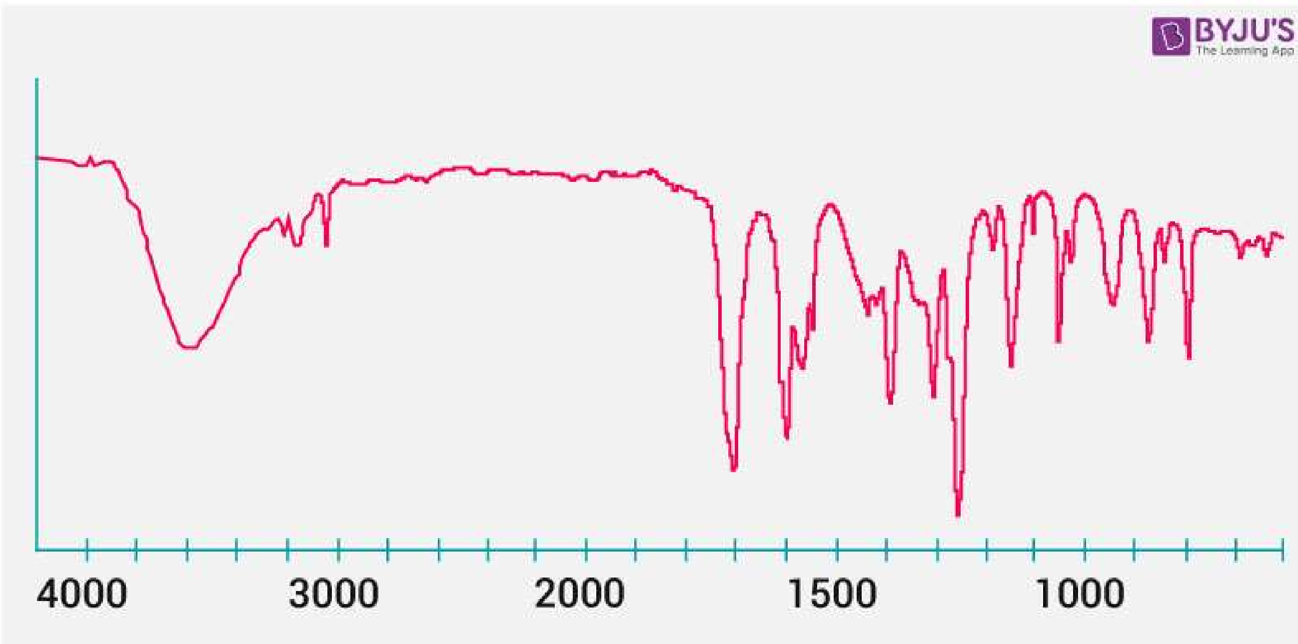
The instrumentation of infrared spectroscopy is illustrated below. First, a beam of IR light from the source is split into two and passed through the reference ant the sample respectively.



Now, both of these beams are reflected to pass through a splitter and then through a detector. Finally, the required reading is printed out after the processor deciphers the data passed through the detector.

Graph of the IR spectrum

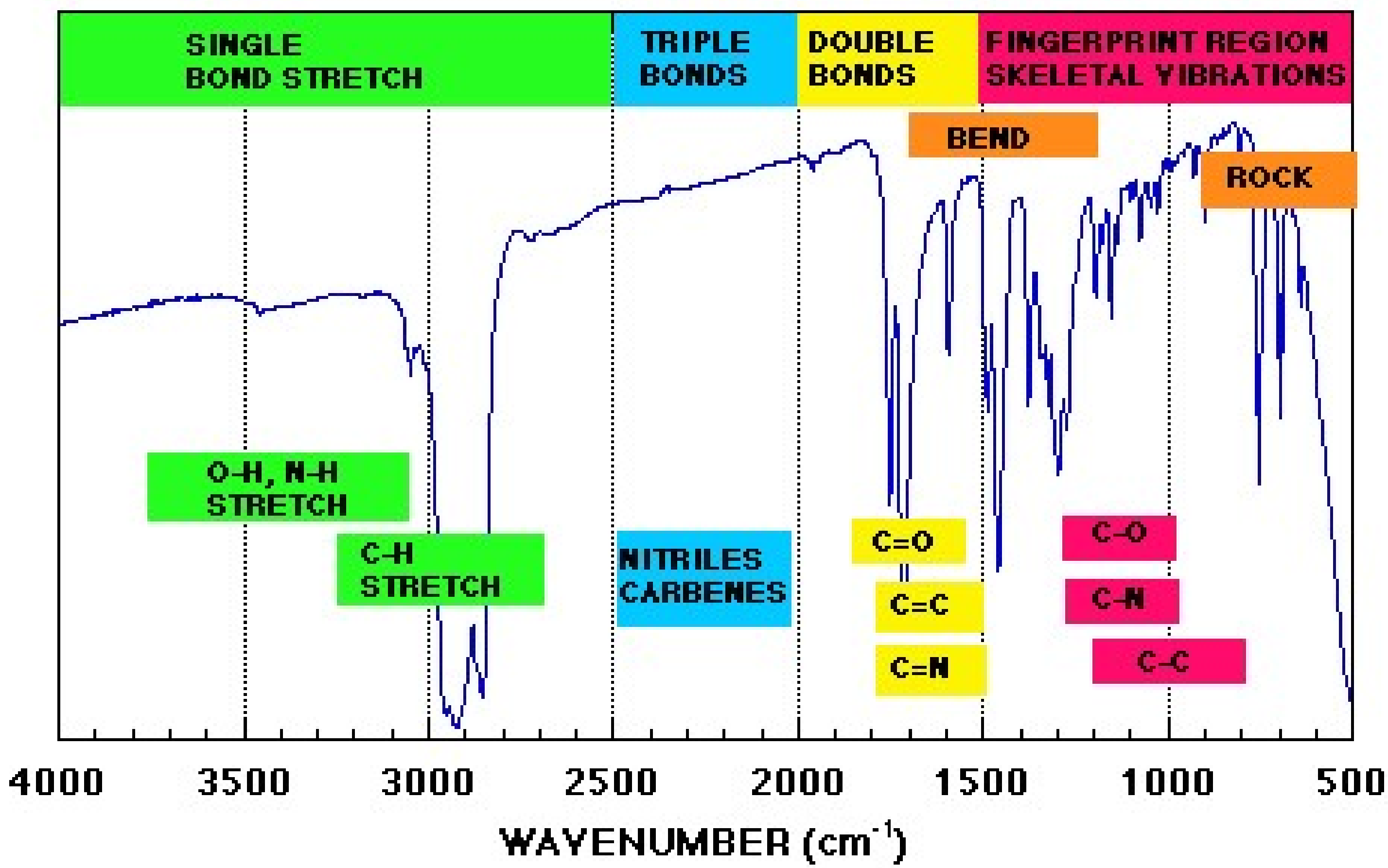
Given below is a sample of typical Infrared Absorption Frequencies.

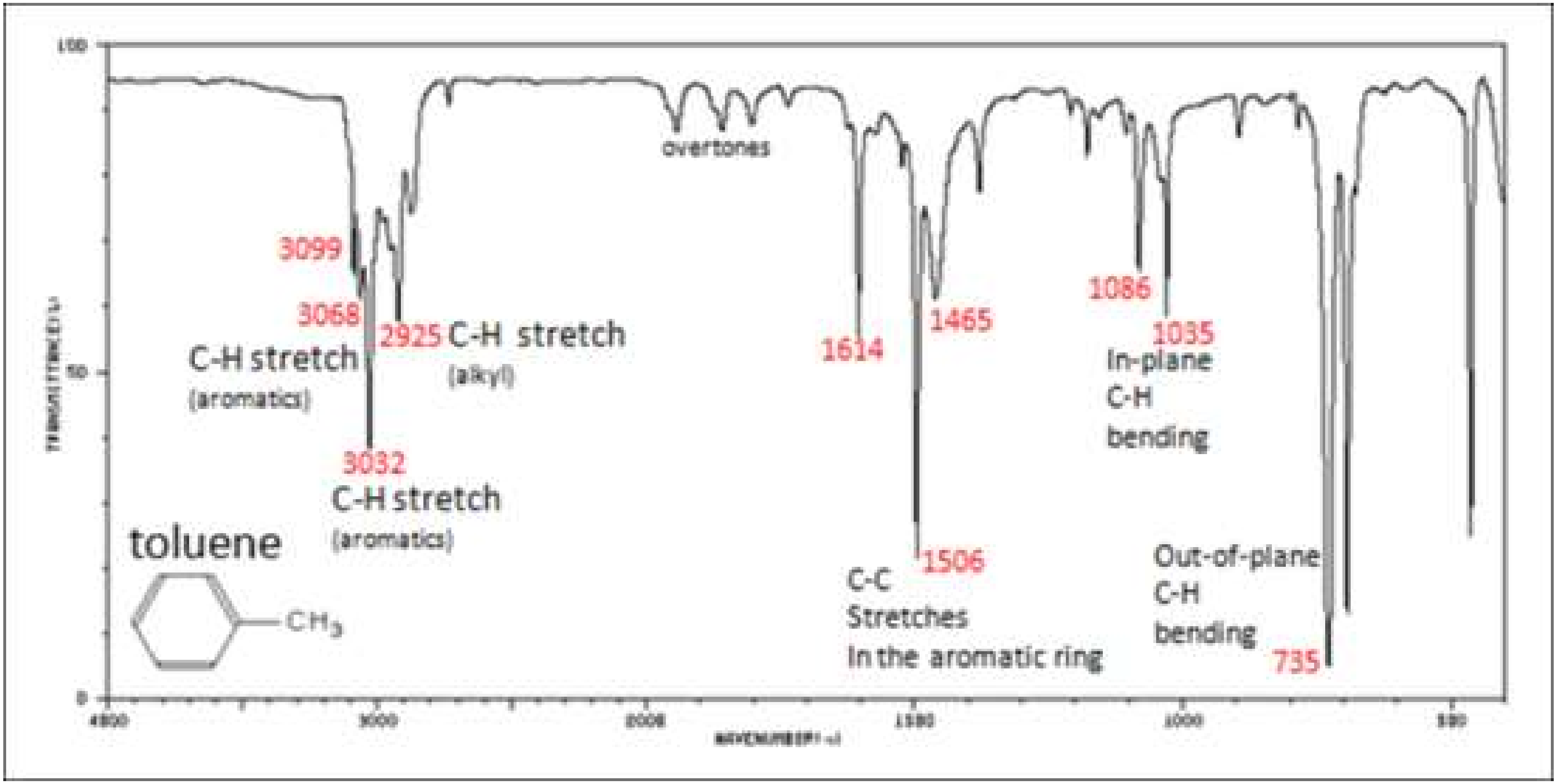


Thus, IR spectroscopy involves the collection of absorption information and its analysis in the form of a spectrum.

TABLE 17-2 Abbreviated Table of Group Frequencies for Organic Groups

Bond	Type of Compound	Frequency Range, cm^{-1}	Intensity
C—H	Alkanes	2850–2970	Strong
		1340–1470	Strong
C—H	Alkenes ($>C{=}C<^{H}$)	3010–3095	Medium
		675–995	Strong
C—H	Alkynes (—C≡C—H)	3300	Strong
C—H	Aromatic rings	3010–3100	Medium
		690–900	Strong
O—H	Monomeric alcohols, phenols	3590–3650	Variable
	Hydrogen-bonded alcohols, phenols	3200–3600	Variable, sometimes broad
	Monomeric carboxylic acids	3500–3650	Medium
	Hydrogen-bonded carboxylic acids	2500–2700	Broad
N—H	Amines, amides	3300–3500	Medium
C═C	Alkenes	1610–1680	Variable
C═C	Aromatic rings	1500–1600	Variable
C≡C	Alkynes	2100–2260	Variable
C—N	Amines, amides	1180–1360	Strong
C≡N	Nitriles	2210–2280	Strong
C—O	Alcohols, ethers, carboxylic acids, esters	1050–1300	Strong
C═O	Aldehydes, ketones, carboxylic acids, esters	1690–1760	Strong
NO_2	Nitro compounds	1500–1570	Strong
		1300–1370	Strong


SINGLE BOND STRETCH
TRIPLE BONDS
DOUBLE BONDS
FINGERPRINT REGION SKELETAL VIBRATIONS
BEND
ROCK
O-H, N-H STRETCH
C-H STRETCH
NITRILES CARBENES
C=O
C=C
C=N
C-O
C-N
C-C
4000
3500
3000
2500
2000
1500
1000
500
WAVENUMBER (cm-1)



overtones
3099
3068
2925 C-H stretch
(alkyl)
C-H stretch
(aromatics)
3032
C-H stretch
(aromatics)
toluene
CH3
1614
1465
1506
C-C
Stretches
In the aromatic ring
1086
1035
In-plane
C-H
bending
Out-of-plane
C-H
bending
735

APPLICATIONS OF IR SPECTROSCOPY

- Identification of functional groups & structure elucidation of organic compounds.
- Quantitative analysis of a number of organic compounds.
- Study of covalent bonds in molecules.
- Studying the progress of reactions.
- Detection of impurities in a compound.
- Ratio of cis-trans isomers in a mixture of compounds.
- Shape of symmetry of an inorganic molecule.
- Study the presence of water in a sample.
- Measurement of paints and varnishes.

Other Applications

1. Determination of unknown contaminants in industry using FTIR.
2. Determination of cell walls of mutant & wild type plant varieties using FTIR.
3. Biomedical studies of human hair to identify disease states (recent approach).
4. Identify odour & taste components of food.
5. Determine atmospheric pollutants from atmosphere itself.