

INFRARED SPECTROSCOPY

(IR)

Theory and Interpretation of IR spectra

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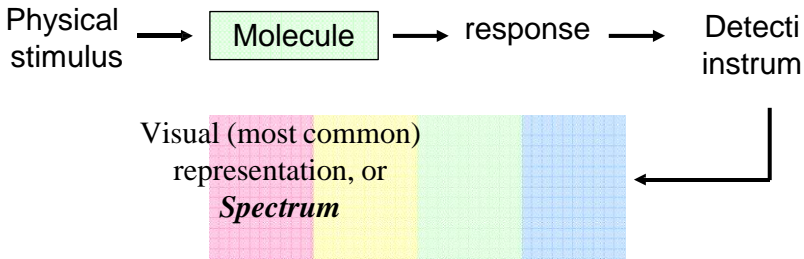
How do we know:

- How atoms are connected together?
- Which bonds are single, double, or triple
- What functional groups exist in the molecule?
- If we have a specific stereoisomer?

STRUCTURE DETERMINATION

1. **Nuclear Magnetic Resonance (NMR)** – Excitation of the nucleus atoms through radiofrequency irradiation. Provides extensive information about molecular structure and atom connectivity.
2. **Infrared Spectroscopy (IR)** – Triggering molecular vibrations through irradiation with infrared light. Provides mostly information about the presence or absence of certain functional groups.
3. **Mass spectrometry** – Bombardment of the sample with electrons and detection of resulting molecular fragments. Provides information about molecular mass and atom connectivity.
4. **Ultraviolet spectroscopy (UV)** – Promotion of electrons to high energy levels through irradiation of the molecule with ultraviolet. Provides mostly information about the presence of conjugated π systems and the presence of double and triple bonds.

information



Upon irradiation with infrared light, certain bonds respon by vibrating faster. This response can be detected and translated into a visual representation called a spectrum

PROCESS

1. Recognize a *pattern*.
2. Associate patterns with *physical parameters*.
3. Identify possible meanings, i.e. *propose explanations*.

Once a spectrum is obtained, the main challenge is to extract the information it contains in abstract, or hidden form. This requires the recognition of certain patterns, the association of these patterns with physical parameters, and the interpretation of these patterns in terms of meaningful and logical explanations.

Most organic spectroscopy uses **electromagnetic energy, or radiation** as the physical stimulus.

Electromagnetic energy (such as visible light) has no detectable mass component. In other words, it can be referred to as “pure energy.”

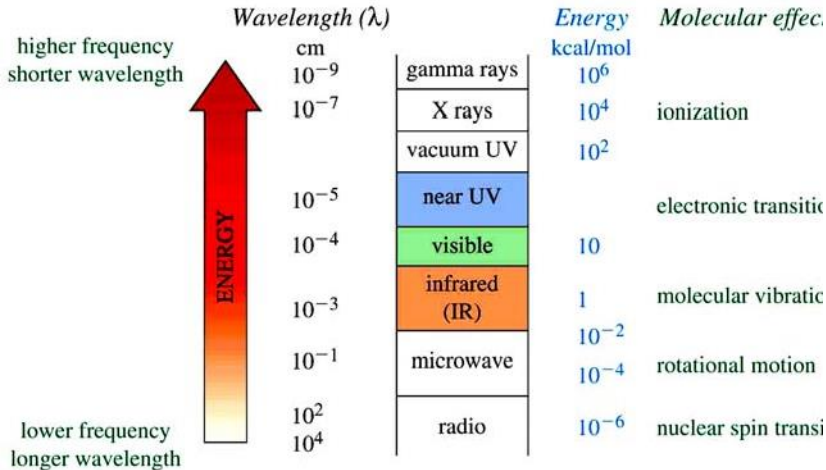
Other types of radiation such as alpha rays, which consist of helium nuclei, have a detectable mass component and therefore cannot be categorized as electromagnetic energy.

The important parameters associated with electromagnetic radiation

- **Energy (E):** Energy is directly proportional to frequency, and inversely proportional to wavelength, as indicated by the equation below.
- **Frequency (ν)**
- **Wavelength (λ)**

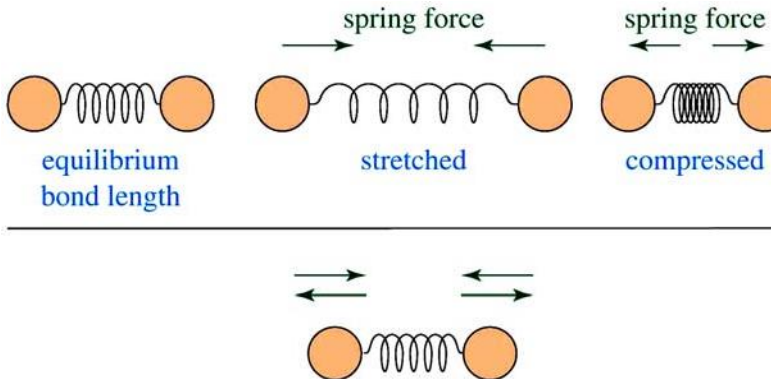
$$E = h\nu$$

ON MOLECULES

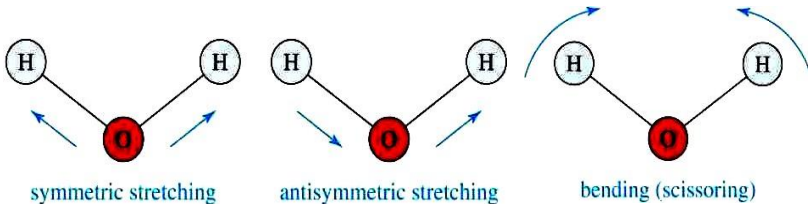


It induces stronger **molecular vibrations** in covalent bonds, which be viewed as springs holding together two masses, or atoms.

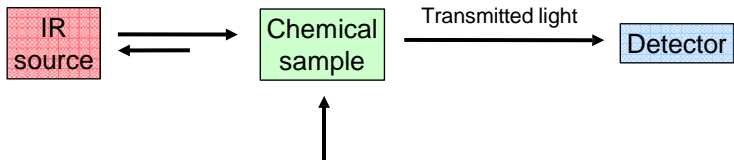
Specific bonds respond to (absorb) **specific** frequencies



- Covalent bonds can vibrate in several modes, including **stretching**, **rocking**, and **scissoring**.
- The most useful bands in an infrared spectrum correspond to stretching frequencies, and those will be the ones we'll focus on.



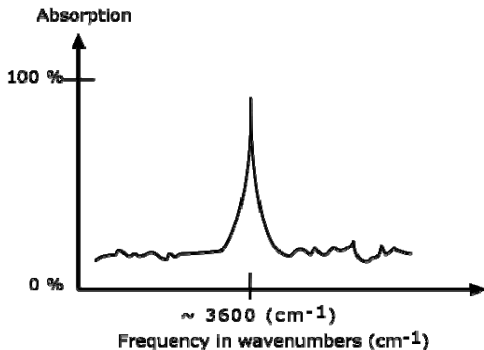
When a chemical sample is exposed to the action of **IR LIGHT**, it can **absorb** some frequencies and **transmit** the rest. Some of the light also be reflected back to the source.



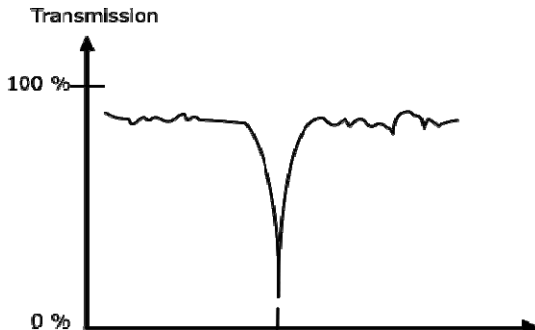
From all the frequencies it receives, the chemical sample can **absorb** (retain) **specific frequencies** and allow the rest to pass through it (transmitted light).

The detector detects the transmitted frequencies, and by doing so also reveals the values of the absorbed frequencies.

The IR spectrum is basically a plot of transmitted (or absorbed) frequency vs. intensity of the transmission (or absorption). Frequencies appear in the x -axis in units of inverse centimeters (wavenumbers), and intensities are plotted on the y -axis in percentage units.

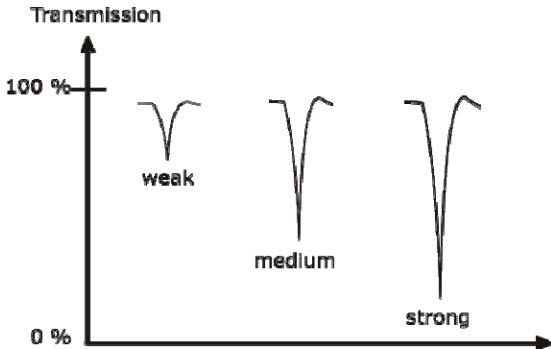


The graph above shows a spectrum in **absorption** mode.



The graph above shows a spectrum in **transmission** mode. **This is the most commonly used representation** and the one found in chemistry and spectroscopy books. Therefore we will use this representation

IR bands can be classified as **strong** (s), **medium** (m), or **weak** (w) depending on their relative intensities in the infrared spectrum. A band covers most of the y-axis. A medium band falls to about half of y-axis, and a weak band falls to about one third or less of the y-axis



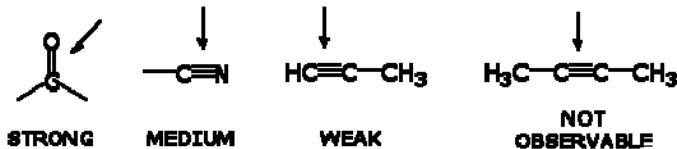
Not all covalent bonds display bands in the IR spectrum.

Only polar bonds do so.

These are referred to as IR active.

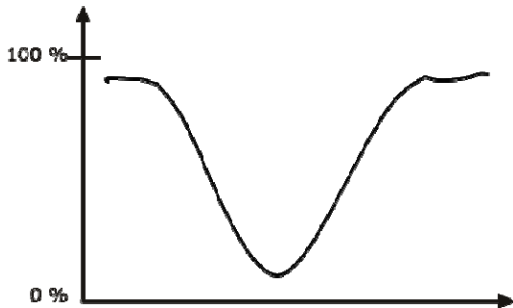
The intensity of the bands depends on the magnitude of the **dipole moment** associated with the bond in question:

- Strongly polar bonds such as carbonyl groups (C=O) produce strong bands.
- Medium polarity bonds and asymmetric bonds produce medium bands.
- Weakly polar bond and symmetric bonds produce weak or non-observable bands.



Infrared band shapes come in various forms. Two of the most common are **narrow** and **broad**. Narrow bands are thin and pointed, like a dagger. Broad bands are wide and smoother.

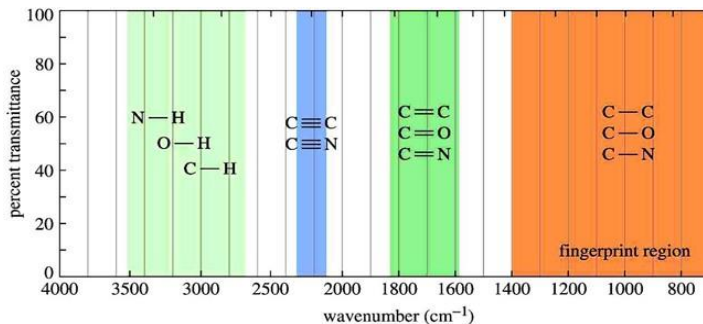
A typical example of a broad band is that displayed by O-H bonds, as those found in alcohols and carboxylic acids, as shown below.



- IR is most useful in providing information about the presence or absence of specific **functional groups**.
- IR can provide a **molecular fingerprint** that can be used when comparing samples. If two pure samples display the same IR spectrum it can be argued that they are the same compound.
- IR **does not** provide detailed information or proof of molecular formula or structure. It provides information on molecular fragments specifically functional groups.
- Therefore it is very limited in scope, and must be used in conjunction with other techniques to provide a more complete picture of the molecular structure.

The typical IR absorption range for covalent bonds is **600 - 4000 cm^{-1}** .

The regions of the spectrum where the following types of bonds normally absorb. For example a sharp band around 2200-2400 cm^{-1} would indicate the possible presence of a C-N or a C-C triple bond.



Thanks