

## Infrared 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. Infrared spectroscopy (IR spectroscopy or vibrational spectroscopy) is the measurement of the interaction of infrared radiation with the matter by absorption, emission, or reflection. It is used to study and identify chemical substances or functional groups in solid, liquid, or gaseous forms. The method or technique of infrared spectroscopy is conducted with an instrument called an infrared spectrometer (or spectrophotometer) which produces an infrared spectrum. An IR spectrum can be visualized in a graph of infrared light absorbance (or transmittance) on the vertical axis vs. frequency or wavelength on the horizontal axis. Typical units of frequency used in IR spectra are reciprocal centimeters (sometimes called wavenumbers), with the symbol  $\text{cm}^{-1}$ . Units of IR wavelength are commonly given in micrometers (formerly called "microns"), symbol  $\mu\text{m}$ , which are related to wave numbers in a reciprocal way. A common laboratory instrument that uses this technique is a Fourier transform infrared (FTIR) spectrometer. Two-dimensional IR is also possible.

The infrared portion of the electromagnetic spectrum is usually divided into three regions; the near-, mid- and far- infrared, named for their relation to the visible spectrum. The higher-energy near-IR, approximately  $14,000\text{--}4,000\text{ cm}^{-1}$  ( $0.7\text{--}2.5\ \mu\text{m}$  wavelength) can excite overtone or combination modes of molecular vibrations. The mid-infrared, approximately  $4,000\text{--}400\text{ cm}^{-1}$  ( $2.5\text{--}25\ \mu\text{m}$ ) is generally used to study the fundamental vibrations and associated rotational-vibrational structure. The far-infrared, approximately  $400\text{--}10\text{ cm}^{-1}$  ( $25\text{--}1,000\ \mu\text{m}$ ) has low energy and may be used for rotational spectroscopy and

low-frequency vibrations. The region from 2–130  $\text{cm}^{-1}$ , bordering the microwave region, is considered the terahertz region and may probe intermolecular vibrations.<sup>[1]</sup> The names and classifications of these subregions are conventions and are only loosely based on the relative molecular or electromagnetic properties.

### **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.

### **Sample preparation**

#### **Gas samples**

Gaseous samples require a sample cell with a long pathlength to compensate for the diluteness. The path length of the sample cell depends on the concentration of the compound of interest. A simple glass tube with a length of 5 to 10 cm equipped with infrared-transparent windows at both ends of the tube can be used for concentrations down to several hundred ppm. Sample gas concentrations well below ppm can be measured with a White's cell in which the infrared light is guided with mirrors to travel through the gas. White's cells are available with optical pathlength starting from 0.5 m up to a hundred meters.

#### **Liquid samples**

Liquid samples can be sandwiched between two plates of a salt (commonly sodium chloride, or common salt, although several other salts such as potassium bromide or calcium fluoride are also used).<sup>[5]</sup> The plates are transparent to the infrared light and do not introduce any lines onto the spectra.

## **Solid samples**

Solid samples can be prepared in a variety of ways. One common method is to crush the sample with an oily mulling agent (usually mineral oil Nujol). A thin film of the mull is applied onto salt plates and measured. The second method is to grind a quantity of the sample with a specially purified salt (usually potassium bromide) finely (to remove scattering effects from large crystals). This powder mixture is then pressed in a mechanical press to form a translucent pellet through which the beam of the spectrometer can pass.<sup>[5]</sup> A third technique is the "cast film" technique, which is used mainly for polymeric materials. The sample is first dissolved in a suitable, non-hygroscopic solvent. A drop of this solution is deposited on the surface of KBr or NaCl cell. The solution is then evaporated to dryness and the film formed on the cell is analyzed directly. Care is important to ensure that the film is not too thick otherwise light cannot pass through. This technique is suitable for qualitative analysis. The final method is to use microtomy to cut a thin (20–100  $\mu\text{m}$ ) film from a solid sample. This is one of the most important ways of analyzing failed plastic products for example because the integrity of the solid is preserved.

In photoacoustic spectroscopy the need for sample treatment is minimal. The sample, liquid or solid, is placed into the sample cup which is inserted into the photoacoustic cell which is then sealed for the measurement. The sample may be one solid piece, powder or basically in any form for the measurement. For example, a piece of rock can be inserted into the sample cup and the spectrum measured from it.

Table : IR absorptions spectra of some common functional groups

IR Absorptions of Common Functional Groups		
Functional Group	Absorption Location ( $\text{cm}^{-1}$ )	Absorption Intensity
Alkane (C-H)	2,850–2,975	Medium to strong
Alcohol (O-H)	3,400–3,700	Strong, broad
Alkene (C=C)	1,640–1,680	Weak to medium
(C=C-H)	3,020–3,100	Medium
Alkyne (C≡C)	2,100–2,250	Medium
(C≡C-H)	3,300	Strong
Nitrile (C≡N)	2,200–2,250	Medium
Aromatics	1,650–2,000	Weak
Amines (N-H)	3,300–3,350	Medium
Carbonyls (C=O)		Strong
Aldehyde (CHO)	1,720–1,740	
Ketone (RCOR)	1,715	
Ester (RCOOR)	1,735–1,750	
Acid (RCOOH)	1,700–1,725	

Example : IR spectra of Ethanoic Acid

