

# An Overview of Infrared Spectroscopy

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## Description

The measurement of the interaction of infrared radiation with matter by absorption, emission, or reflection is known as infrared spectroscopy (IR spectroscopy or vibrational spectroscopy). It's utilised to investigate and identify chemical compounds or functional groups in solid, liquid, or gaseous states. It can be used to identify and validate known and unknown samples, as well as to characterise new materials. Infrared spectroscopy is a method or technique that uses equipment called an infrared spectrometer (or spectrophotometer) to obtain an infrared spectrum. A graph of infrared light absorbance (or transmittance) on the vertical axis vs. frequency or wavelength on the horizontal axis can be used to visualise an IR spectrum. The symbol  $\text{cm}^{-1}$  stands for reciprocal centimetres (also known as wave numbers) in infrared spectra. IR wavelengths are generally expressed in micrometres (previously "microns"), symbol  $\mu\text{m}$ , which are reciprocally connected to wave numbers. A Fourier transform infrared (FTIR) spectrometer is a common laboratory device that employs this technology. As explained below, two-dimensional IR is also achievable [1].

The near-, mid-, and far-infrared portions of the electromagnetic spectrum are commonly split into three sections based on their relationship to the visible spectrum. Near-IR light with a wavelength of  $14,000\text{--}4,000\text{ cm}^{-1}$  ( $0.7\text{--}2.5\text{ }\mu\text{m}$ ) can excite overtone or combination modes of molecular vibrations. The mid-infrared, which ranges from  $4,000\text{ to }400\text{ cm}^{-1}$  ( $2.5\text{--}25\text{ }\mu\text{m}$ ), is commonly employed to investigate basic vibrations and their accompanying rotational-vibrational structure. The far-infrared has a low energy range of  $400\text{--}10\text{ cm}^{-1}$  ( $25\text{--}1,000\text{ }\mu\text{m}$ ) and can be used for rotational spectroscopy and low frequency vibrations. The terahertz range, which extends from  $2\text{ to }130\text{ cm}^{-1}$  and borders the microwave zone, can be used to study intermolecular vibrations. These subregions' names and classifications are conventions that are only loosely based on relative chemical or electromagnetic properties [2].

The fact that molecules absorb frequencies that are distinctive of their structure is exploited in infrared spectroscopy. These absorptions happen at resonance frequencies, which mean the absorbed radiation frequency is the same as the vibrational frequency. The form of the molecular potential energy surfaces, the masses of the atoms and the accompanying vibronic coupling all influence the energies.

The resonant frequencies are associated with the normal modes of vibration corresponding to the molecular electronic ground state potential energy surface in the Born-Oppenheimer and harmonic approximations, i.e. when the molecular Hamiltonian corresponding to the electronic ground state can be approximated by a harmonic oscillator in the neighbourhood of the equilibrium molecular geometry. The resonance frequencies are also affected by the bond's strength and the mass of the atoms on either end. As a result, the vibration frequency is linked to a specific normal mode of motion and a specific bond type [1].

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## Number of vibrational modes

A vibrational mode in a sample must be connected with variations in the dipole moment in order to be "IR active." The rule simply requires a change in dipole moment; hence no permanent dipole is required.

A molecule can vibrate in a variety of ways, each of which is referred to as a vibrational mode. Linear molecules have  $3N-5$  degrees of vibrational modes, whereas nonlinear molecules have  $3N-6$  degrees of vibrational modes for molecules with  $N$  atoms (also called vibrational degrees of freedom). The non-linear molecule  $\text{H}_2\text{O}$ , for example, has  $3 \times 3 - 6 = 3$  degrees of vibrational freedom, or modes.

Only one bond and one vibrational band exist in simple diatomic molecules. If the molecule is symmetrical, such as  $\text{N}_2$ , the band is only visible in the Raman spectra, not the IR spectrum. CO and other asymmetrical diatomic compounds absorb in the infrared spectrum. Because more complex compounds have more bonds, their vibrational spectra are also more complex, resulting in more peaks in their IR spectra [3].

## Practical IR spectroscopy

A sample's infrared spectrum is recorded by passing an infrared light beam through it. Absorption occurs when the IR frequency matches the vibrational frequency of a bond or cluster of bonds. The amount of energy absorbed at each frequency can be determined by examining the transmitted light (or wavelength). A monochromator can be used to scan the wavelength range and make this measurement. Alternatively, a Fourier transform device can be used to measure the complete wavelength range, and then a dedicated process can be used to construct a transmittance or absorbance spectrum [4].

**Sample preparation:** To compensate for the diluteness of gaseous samples, a sample cell with a long pathlength is required. The sample cell's pathlength is determined by the concentration of the substance of interest. For concentrations as low as a few hundred ppm, a simple glass tube with a length of  $5\text{ to }10\text{ cm}$  and infrared-transparent windows on both ends can be employed. A White's cell, in which infrared light is steered through the gas by mirrors, may quantify sample gas concentrations much below ppm. White's cells have optical pathlengths ranging from  $0.5\text{ m}$  to several hundred metres.

**Liquid samples:** Samples of liquid can be sandwiched between two salt plates (commonly sodium chloride, or common salt, although a number of other salts such as potassium bromide or calcium fluoride are also used). The plates are infrared light transparent and do not introduce lines into the spectra.

**Solid samples:** Solid samples can be made in a number of different methods. Crushing the sample with an oily mulling agent is a popular approach (usually mineral oil Nujol). On salt plates, a thin film of mull is placed and measured. The second approach is carefully grinding a portion of the sample with a particularly purified salt (often potassium bromide) (to remove scattering effects from large crystals). After that, the powder mixture is squeezed in a mechanical press to form a translucent pellet through which the spectrometer's beam can pass. The "cast film" approach is a third technique that is mostly employed for polymeric materials. First, the material is dissolved in a non-hygroscopic solvent. On the surface, a drop of this solution is deposited [5].

## Uses and application

- Infrared spectroscopy is a common technique in organic and inorganic chemistry, as well as in research and industry. It is a very important instrument in catalysis research for characterising the catalyst, as well as detecting intermediates and products throughout the catalytic reaction. Infrared gas analyzers are utilised in quality control, dynamic

measurement, and monitoring applications such as long-term unattended CO<sub>2</sub> concentration measurements in greenhouses and growth chambers.

- It's also employed in forensic analysis, both criminal and civil, to determine polymer degradation, for example. It can be used to determine a suspected drunk driver's blood alcohol content.
- Infrared spectroscopy has been used to analyse and identify pigments in paintings and other art objects, such as illuminated manuscripts.
- ATR, or attenuated total reflectance spectroscopy, is a useful means of studying solid samples without having to cut them. Samples are rubbed against the face of a single crystal in this method. Infrared radiation travels through the crystal and only interacts with the sample at the material's interface.
- Infrared spectroscopy has also been effectively applied to semiconductors such as silicon, gallium arsenide, gallium nitride, zinc selenide, amorphous silicon, silicon nitride, and other semiconductors.

## Conclusion

IR spectroscopy is extremely sensitive to RNA conformational changes. The IR spectrum of an RNA molecule exhibits many absorption transitions, each of which can be assigned to a specific molecular group of the RNA. If considered individually, each transition would provide a useful metric

to monitor conformational changes. However, it is the ability to monitor the collective response of several transitions simultaneously that is unique to IR spectroscopy. Doing so allows for a more detailed analysis of structural changes. Moreover, folding kinetics can be studied by monitoring the IR spectrum as a function of time following a rapid laser-induced T-jump.

## Conflict Of Interest

None.

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