

Infrared Absorption Spectroscopy

3.1 Introduction

Infrared spectroscopy is one of the most powerful analytical techniques which offers the possibility of chemical identification. This technique when coupled with intensity measurements may be used for quantitative analysis. One of the most important advantages of infrared spectroscopy over the other usual methods of structural analysis (X-ray diffraction, electron spin resonance, etc.) is that it provides useful information about the structure of molecule quickly, without tiresome evaluation methods. This method can solve many problems in organic chemistry and coordination chemistry, while in some other problems infrared data advantageously complement the results obtained by other methods.

Infrared spectroscopy has established itself as a valuable tool for the determination of organic, and to a lesser extent, inorganic, structure. The utilization of infrared data in conjunction with other physical measurements, such as those obtained from nuclear magnetic resonance and mass spectroscopy, has elucidated many facts about the structure and properties of organic compounds, facts which were heretofore accepted solely on a theoretical basis.

Infrared spectroscopy may be applied at all levels of expertise from a simple matching of spectra on one end to theoretical calculations at the other. The instruments are common, relatively inexpensive, and easy to operate. This, combined with the non-destructive nature of the analysis, means that records on intermediate preparative or separation products may be easily obtained. The sample may then be recovered and further utilized. While qualitative applications are most common, the absorption of infrared radiation does follow Beer's Law and therefore lends itself to quantitative determinations.

The technique is based upon the simple fact that a chemical substance shows marked selective absorption in the infrared region. After absorption of IR radiations, the molecules of a chemical substance vibrate at many rates of vibration, giving rise to close-packed absorption bands, called an IR *absorption spectrum* which may extend over a wide wavelength range. Various bands will be present in a chemical substance, which will correspond to the characteristic functional groups and bonds present in a chemical substance. Thus, an IR spectrum of a chemical substance is a fingerprint for its identification.

Band positions in an infrared spectrum may be expressed conveniently by the wave number $\bar{\nu}$, whose unit is cm^{-1} . The relation between wave number $\bar{\nu}$, wavelength λ and frequency ν is as follows

$$\nu = c/\lambda$$

$$\bar{\nu}(\text{cm}^{-1}) = \nu/c = 1/\lambda$$

where c is the velocity of light. From the above relations, it follows that wave number is the reciprocal of wavelength.

Band intensities in IR spectrum may be expressed either as transmittance (T) or absorbance (A). Transmittance is defined as the ratio of radiant power transmitted by a sample to the radiant power incident on the sample. On the other hand, absorbance is defined as the logarithm, to the base, 10, of the reciprocal of the transmittance, i.e.,

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