

Infra-red Spectroscopy

Infra-red (IR) spectroscopy is based on the principle that the various structural features of a molecule will each absorb infra-red radiation at quite precisely defined frequencies which are characteristic of the particular structural features. In practice the sample (which may be a solid, liquid, solution or vapour) in a suitable form is irradiated with broad-band infra-red radiation and the amount of radiation absorbed at various frequencies (or more usually the derived wavelengths or wavenumbers) is measured. The output is an IR spectrum in which absorption is plotted as a function of wavelength (or wavenumber); this IR spectrum is quite characteristic of the compound under investigation and no other compound will have a completely identical spectrum. A recent major advance in IR spectroscopy is the development of Fourier Transform (FT) infra-red spectroscopy, commonly abbreviated FTIR. The Fourier Transform technique is basically a mathematical means of manipulating the signal, which is in the form of an interferogram, so that all the energy recoverable from the sample is actually utilised in the generation of the signal. This has the following two immediate practical advantages:

- a) By utilising all of the recoverable energy the time taken to measure a spectrum is greatly reduced, typically from about five minutes on a dispersion instrument down to one second on a FTIR instrument, so the measurement is much more rapid.
- b) Utilising the total recoverable energy from the sample also improves the sensitivity compared with a dispersion instrument. This improvement is typically of the order of 50 times for scan times of about one second but can be further improved if longer scan times, involving a larger number of FT accumulations, are used; with scan times of one hour sensitivities, in favourable cases, in the nanogram range can be obtained.

IR spectroscopy (and FTIR) is an excellent technique for confirming the identity of known compounds when either an authenticated reference sample of the same material is available for a comparison spectrum to be measured; alternatively the measured spectrum may be compared directly with an authenticated reference spectrum previously measured on a fully authenticated sample and which may be available for comparison purposes either as hard copy or, more frequently now, on a computerised data base.