

IR spectroscopy alone can rarely give unambiguous full structure elucidation on unknown compounds except in very favourable cases, but when used in conjunction with techniques such as Nuclear Magnetic Resonance (NMR) and Mass Spectrometry it can provide very useful structural data particularly on the functional groups present in an unknown compound the structure of which needs to be elucidated.

Due to the very rapid scan times available with FTIR it is now possible, as with mass spectrometry, to integrate FTIR with chromatographic separation techniques such as gas chromatography. Complex mixtures can then be resolved into their individual components by the chromatographic technique and as the separated components emerge as peaks from the chromatographic column they are scanned by the FTIR to produce an IR spectrum of that particular component free from any interference by the other components of the mixture. Such an integrated GC-FTIR instrument makes use of both of the particular advantages of FTIR namely rapid scan times and increased sensitivity. Further increase in sensitivity is obtained if the eluting peaks can be frozen onto the cold surface enabling extended scan times. High resolution obtained with the matrix isolation technique further lowers the detection limit to picogram level.

Nuclear Magnetic Resonance (NMR) Spectroscopy

NMR spectroscopy is a technique which uses a radio frequency field to interrogate the interactions of a powerful applied magnetic field with the local magnetic environments within molecules containing particular atomic nuclei (for example ^1H , ^{31}P , ^{19}F and ^{13}C). The technique yields spectra which, by appropriate skilled interpretation, can yield very detailed information on the way in which the various atoms in the molecule are linked to each other and on their relative dispositions in 3-dimensional space. Although the original continuous wave instruments are being largely displaced by Fourier Transform Instruments (FTNMR) the latter, although having much shorter scan times, still do not by any means have the sensitivity achieved by either mass spectrometry or FTIR techniques.

NMR spectroscopy is well suited to the identification of known compounds; the identifications can be confirmed either by comparison of the measured spectrum with the spectrum, measured under identical conditions, of an authentic sample of the same compound or by comparison of the spectrum with an authenticated reference spectrum either as hard copy or in a computerised data bank of NMR spectra. It is also an important technique for the validation and authentication