HL Analytical techniques and the principles of spectroscopy

INFORMATION FROM DIFFERENT ANALYTICAL TECHNIQUES

This option builds on some of the techniques that have already been mentioned in 11. Topic 20 – Organic Chemistry. Techniques such as ultraviolet/visible spectroscopy, infrared spectroscopy, mass spectrometry, and nuclear magnetic resonance spectroscopy are extremely useful tools to chemists. They are becoming ever more refined and some of them (e.g. mass spectrometry) can be used on extremely small samples. This has revolutionized many branches of chemistry, for example combinatorial chemistry in the search for new drugs. This is only possible because very small amounts of thousands of new compounds can be analysed accurately and efficiently.

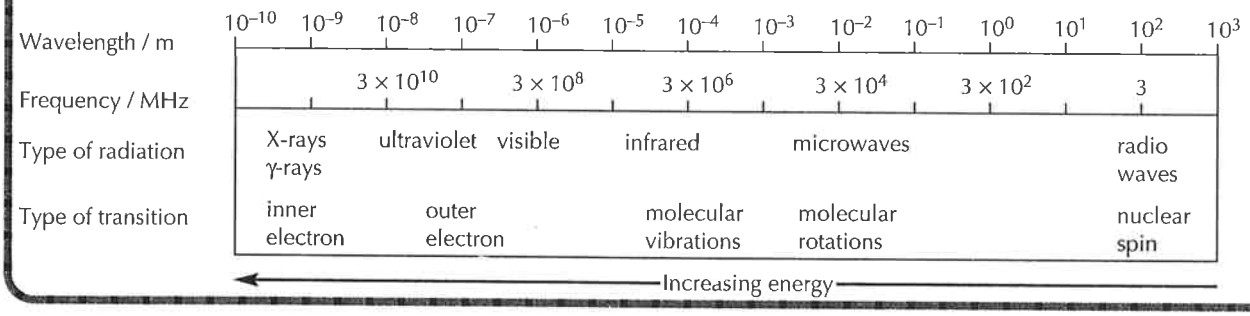
The main uses for these techniques are structural determination, the analysis of the different composition of compounds, and to determine purity. Before analysis can usually take place it is important to separate any mixture into its individual components – hence the need for chromatography. Often information is not obtained from a single technique but from a combination of several of them. Some examples are:

- Ultraviolet and visible spectroscopy – assaying of metal ions, organic structural determination, and detection of drug metabolites.
- Infrared spectroscopy – organic structural determination, information on the strength of bonds, information about the secondary structure of proteins, measuring the degree of unsaturation of oils and fats, and determining the level of alcohol in the breath.
- Mass spectrometry – organic structural determination, isotopic dating (e.g. ^{14}C dating).
- ^{1}H nuclear magnetic resonance – organic structural determination, body scanning.
- Gas chromatography – mass spectrometry (GC–MS) – drug testing in the blood and urine, food testing, and forensic science.

THE ELECTROMAGNETIC SPECTRUM

The electromagnetic spectrum has already been briefly described in 2. Topic 2 – Atomic Theory. You should be familiar with the relationship $c = \lambda f$ and know the different regions of the spectrum.

The electromagnetic spectrum



ABSORPTION SPECTRA AND EMISSION SPECTRA

Spectroscopy can be divided into two main types. Emission spectroscopy involves the analysis of light emitted by excited atoms or molecules as they return to their ground state. The atomic emission spectrum of hydrogen is a good example of this. Many analytical techniques involve absorption spectroscopy. When radiation is passed through a sample some of the energy is absorbed by the sample to excite an atom or molecule to an excited state. The spectrometer analyses the transmitted energy relative to the incident energy. Since the energy levels are quantized only radiation with a frequency corresponding to the difference in the energy levels will be absorbed. The relationship between energy and frequency is given by:

$E = hf$ where h is Planck's constant, 6.626×10^{-34} J s.

The greater the energy difference between the levels the higher the frequency (or the shorter the wavelength) of the light absorbed. The most energetic absorptions are atomic electronic transitions which involve bond breaking and ionization. Absorptions in the ultraviolet and visible region are due to atomic and molecular transitions in which electrons become excited to higher levels. Molecular vibrations (stretching and bending) occur in the infrared region and molecular rotations in the microwave region. The weakest transitions of all involve nuclear spin. These occur in the radio wave region and form the basis of nuclear magnetic resonance spectroscopy.