

AN6**APPLICATIONS - X-RAYS & NMR****OBJECTIVES****Aims**

Firstly, you should aim to be able to explain how x-rays are produced and the main features of x-ray spectra. You should be able to explain those features. Secondly, you should aim to understand, qualitatively, the physical principles of nuclear magnetic resonance.

Minimum learning goals

When you have finished studying this chapter you should be able to do all of the following.

1. Explain, use and interpret the terms
x rays, x-ray tube, continuous spectrum, cut-off wavelength, characteristic x rays, Moseley's law, nuclear magnetic resonance [NMR], NMR spectroscopy, NMR imaging [MRI].
2. Describe and explain how x rays are produced in an x-ray tube.
3. Sketch typical plots of x-ray spectra for various accelerating voltages.
4. (a) Describe and explain the origin of the continuous x-ray spectrum.
(b) Explain the short wavelength cut-off to the continuous spectrum.
(c) State and apply the relation between the cut-off wavelength and the accelerating voltage (equation 5.1).
5. Explain how characteristic x rays are produced.
6. Describe the principles of NMR, NMR spectroscopy and NMR imaging.

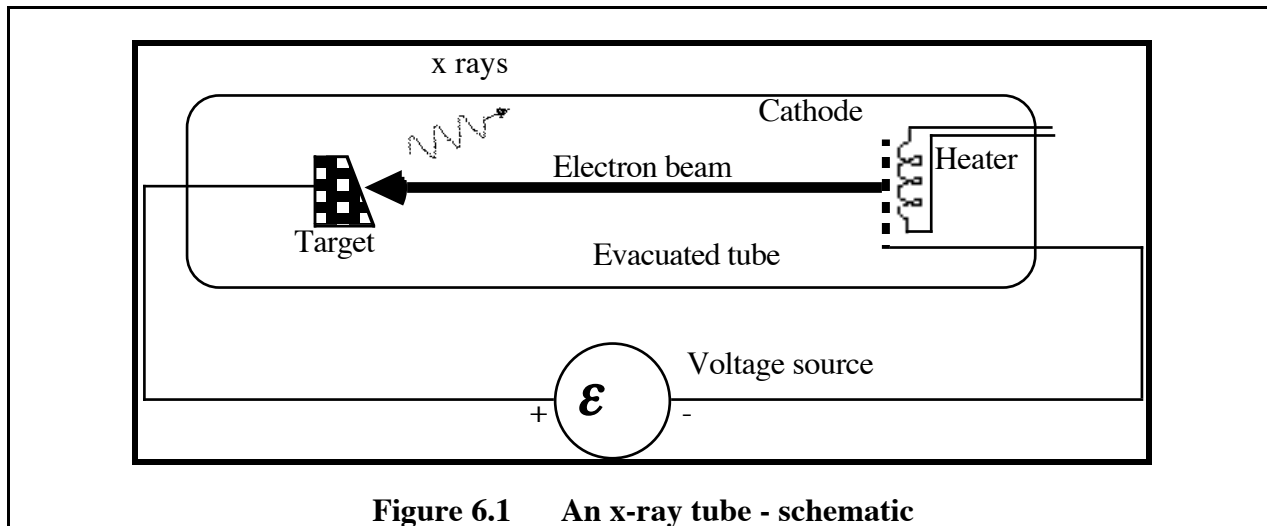
TEXT**6-1 X RAYS**

X rays can be described as very energetic photons or short wavelength electromagnetic radiation. They can be produced when fast charged particles (generally electrons) are stopped by matter. Although x rays and gamma rays can have similar energies, the term gamma rays is usually reserved for radiation produced by the decay of excited nuclei.

X rays were discovered by Wilhelm Röntgen in 1895, while he was investigating electrical discharges through gases. Within five years the discovery had already been applied in many areas of the life sciences. Besides the well-known use for examination of fractured and broken bones, very early attempts were made to apply them to cancer treatment.

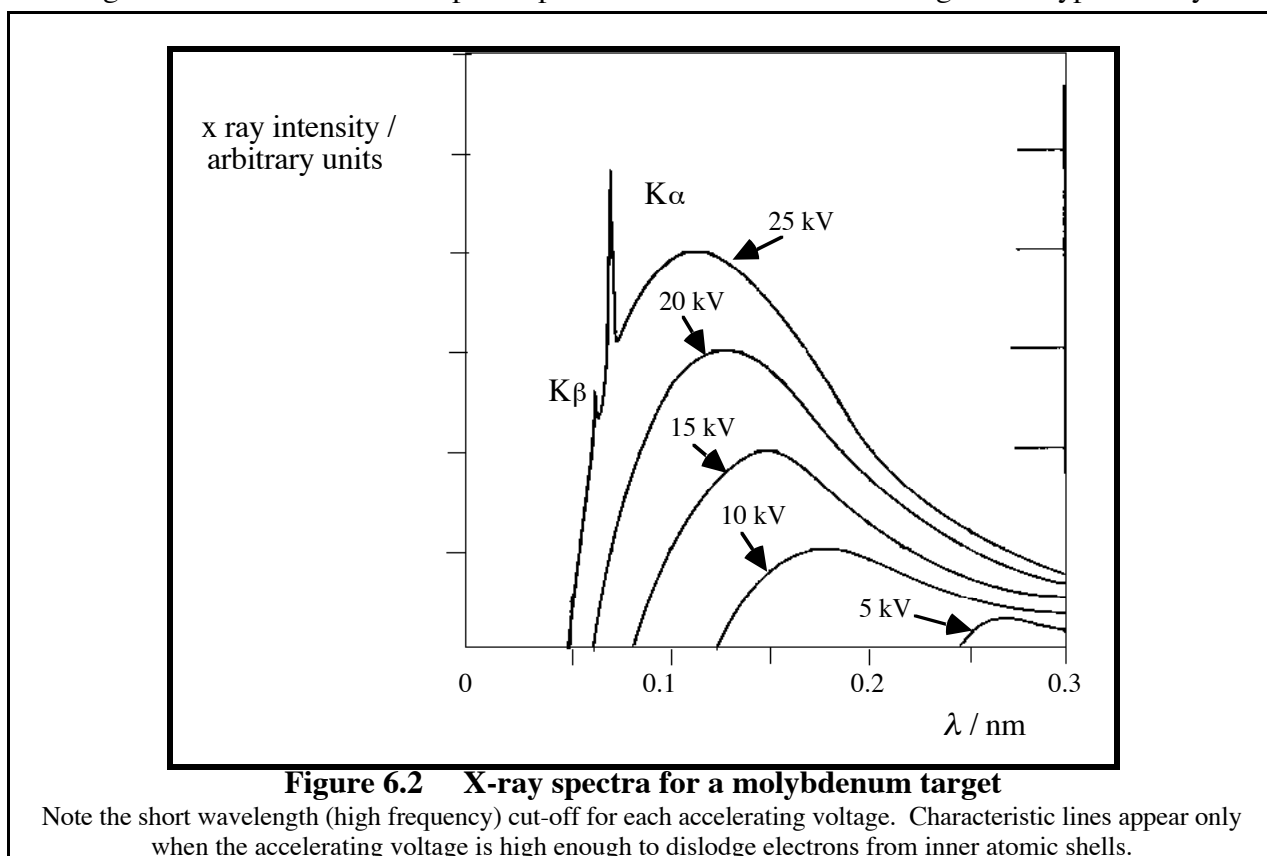
6-2 PRODUCTION OF X RAYS

In an x-ray tube, a beam of electrons is accelerated through a potential difference in the range 10 kV to 200 kV. The electrons then collide with a target of a heavy metallic element such as tungsten or molybdenum. See figure 6.1. Most of the energy of the electron beam goes into increasing the internal (thermal) energy of the target but a small fraction appears as high energy photons - x rays.



6-3 X-RAY SPECTRA

The energies of the x-ray photons, and hence the wavelengths of the radiation, are spread over a range of values. Figure 6.2 shows the radiated power plotted as a function of wavelength for a typical x-ray tube.



For lower values of the accelerating voltage and electron energy, the distribution of x-ray intensity with wavelength is a **continuous spectrum** which cuts out sharply at a fixed value of the wavelength at the short wavelength or high frequency end of the spectrum. (See the curves labelled 5 kV, 10 kV, 15 kV and 20 kV in figure 6.2.) If the accelerating voltage is increased this short wavelength cut-off decreases.

There is also an increase in the total x-ray power and a decrease in the average wavelength. At sufficiently high electron energies, a set of **characteristic lines** may be superimposed on the continuous spectrum. These lines always occur at the same wavelengths for a fixed target material.

Continuous spectrum

In an x-ray tube the electrons are first accelerated by a potential difference V , which gives each of them a kinetic energy eV . About 99% of the electrons that strike the target do nothing spectacular at all. Most of them undergo multiple collisions with the electrons and atoms in the target and, in the course of these collisions, the electrons lose their energy a little at a time and thus merely increase the average kinetic energy of the particles in the target. Thus most of the energy of the electron beam goes into heating the target and the temperature of the target increases. X rays are produced by a few of the fast electrons which penetrate target atoms sufficiently to experience the very strong electric fields near the atomic nuclei. These electrons are strongly accelerated so they can lose most of their energy in one collision by the process of bremsstrahlung - as described in chapter AN4.

Cut-off wavelength

The short wavelength cut-off to the continuous spectrum can be explained as follows. An electron cannot lose more kinetic energy in a collision than it started with, and so the maximum energy of the photons produced is equal to eV . We can work out the highest frequency f_0 (and shortest wavelength λ_0) of the radiation produced. The maximum energy of an x-ray photon is equal to the kinetic energy of one electron which loses all its energy to the photon, so

$$E = eV = hf_0 = \frac{hc}{\lambda_0} ;$$

and the cut-off wavelength is $\lambda_0 = \frac{hc}{eV}$... (6.1).

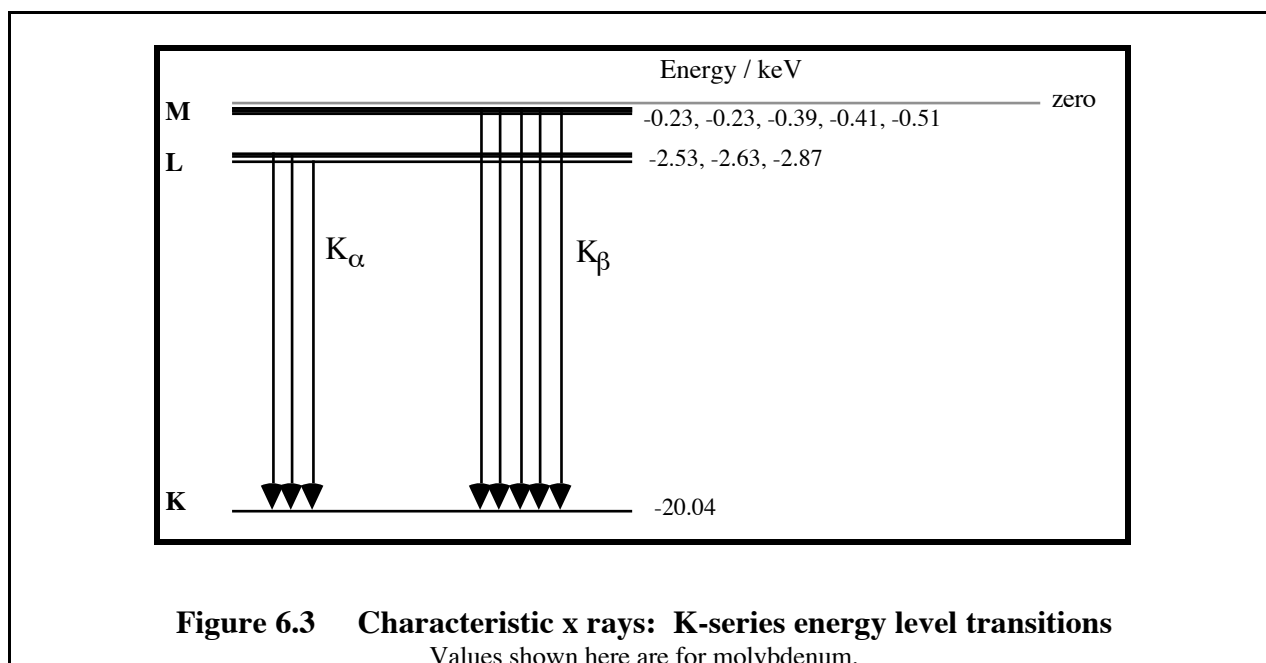
However most of the electrons hitting the target do not lose all their kinetic energy in one hit. An electron might undergo several collisions before emitting an x-ray photon, so the photon's energy will be less than the maximum value. Note that the commonest value of the photon energy is somewhat less than the maximum value, giving a peak intensity at a wavelength greater than the cut-off wavelength.

Characteristic lines

If the accelerating voltage is high enough an x-ray line spectrum can be produced. The line spectrum appears as a set of spikes superimposed on the continuous spectrum, like the 25 kV curve in figure 6.2. The spikes, or lines, indicate that a very large number of x-ray photons of definite wavelength (and hence definite energy) are being emitted. The wavelengths of the lines are characteristic of the material of the target so the radiation is called **characteristic x rays**.

The origin of characteristic x rays can be understood in terms of energy levels within the atoms of the target material. The electrons in the outermost shell, which are responsible for the chemistry of the atom, are only loosely bound. It takes only a few electronvolts to remove one of them to ionise the atom. On the other hand, for example, it takes 20 keV to remove a K-shell electron from a molybdenum atom. This much higher binding energy occurs because K-shell electrons are, on average, closer to the nucleus than those in outer shells and also because electrons in the outer shells are, to some extent, shielded from the attractive electrostatic force of the positive nucleus by the inner electrons.

A characteristic x-ray photon is produced when an accelerated electron knocks an electron out of an inner shell in the target atom and another electron subsequently falls into the vacancy. The excess energy of this third electron is emitted as an x-ray photon.



When electrons fall into the vacancies in the K shell, they produce the **K series** of characteristic x rays. There is a series of lines because the electron which fills the vacancy can come from the L shell, the M shell, the O shell, etc. or even from outside the atom. Within a particular series, transitions are labelled with Greek letters. Figures 6.2 and 6.3 show the K_{α} and K_{β} lines for molybdenum. The single spike labelled K_{α} in the spectrum of figure 6.2 corresponds to a group of three transitions in figure 6.3. Each of the K_{α} and K_{β} lines is really a set of closely spaced lines, corresponding to the slight differences in energy levels within the L and M shells. (The label K_{β} corresponds to the electron falling from the M shell; the K_{α} from the L shell.) Note that in the case of molybdenum, if the accelerating voltage is less than 20.04 kV, no electron can be removed from the K shell so the K_{α} and K_{β} radiation will not be seen. If an electron is knocked out of the L shell we get the L series of lines, produced by electrons falling from outer shells. (No L series lines appear in figure 6.2 only because their wavelengths are off the scale.)

Because the spacing of the energy levels depends on the particular element, the x-ray spectrum is characteristic of the element (just as is its optical spectrum which corresponds to rearrangements among the higher energy levels, or outer shells, where the energy spacing between levels is much smaller). The frequency of characteristic x rays is described by a simple law called Moseley's law. It states that the frequencies of corresponding x-ray spectral lines (such as the K_{α} 's), as we go from element to element, may be represented by an equation of the form

$$f = A(Z - \sigma)^2 \quad \dots (6.2)$$

where Z is the atomic number of the element (the number of protons in the nucleus) and the constants A and σ depend on the particular line (i.e. they have one value for the K_{α} line, another for the K_{β} etc.). For K_{α} and K_{β} we have, approximately,

$$A \approx 2.5 \times 10^{15} \text{ Hz}; \quad \sigma \approx 1.$$

The frequency of a particular line (say the K_{α}) for a particular element depends only on the spacing between the energy levels involved (for the K_{α} line they are the K and L levels). Moseley's law really tells us about how the spacing of corresponding energy levels depends on Z , the atomic number. In the modern theory of the atom, quantum mechanics, Moseley's law can be derived from basic principles.

6-4 X-RAY ENERGIES

X rays can have a large range of energies, from around 100 keV produced in a Van der Graaff machine, to a high energy limit of around 20 GeV produced in the 3 km long linear accelerator at Stanford, U.S.A. Sometimes these high energy x rays are called gamma rays, but that is just a matter of nomenclature - they are all high energy photons.

The energy, frequency and wavelength of some typical x rays and, for comparison, light are shown in the table.

Photon	Energy	Frequency	Wavelength
high energy x ray	1.00 MeV	2.42×10^{20} Hz	1.24×10^{-12} m
low energy x ray	100 eV	2.42×10^{16} Hz	1.24×10^{-8} m
light	2.8 eV	6.7×10^{14} Hz	4.5×10^{-7} m

Table 6.1 X-ray energies

6-5 NUCLEAR MAGNETIC RESONANCE

Since the discovery of magnetism, there have been arguments about whether magnetic fields play any direct role in life. Deleterious effects, as well as quack cures and treatments, have been (and still are) attributed to magnetism. The place of magnetism in such things as water divining and bird migration is, surprisingly, still controversial, while some bacteria (e.g. *Aquaspirillum magnetotacticum*) certainly follow the terrestrial magnetic field to their food. In any discussion of the relevance of magnetism in the life sciences today, one application stands head and shoulders over all rivals: **nuclear magnetic resonance (NMR)**. Both in its potential for biochemical analysis and diagnostic medical imaging, NMR is likely to become one of the most powerful tools ever developed. NMR machines will be commonplace in hospitals within a decade.

Principles of NMR

All atomic isotopes with an odd number of nucleons in the nucleus (^1H , ^{13}C and ^{31}P are biologically significant examples) have a fixed naturally occurring magnetic moment. They behave like tiny bar magnets. In strong magnetic fields such nuclei can, in accordance with the laws of quantum mechanics, take up only a limited number of possible orientations. The proton (^1H) for example, can be aligned only parallel or antiparallel with the field.

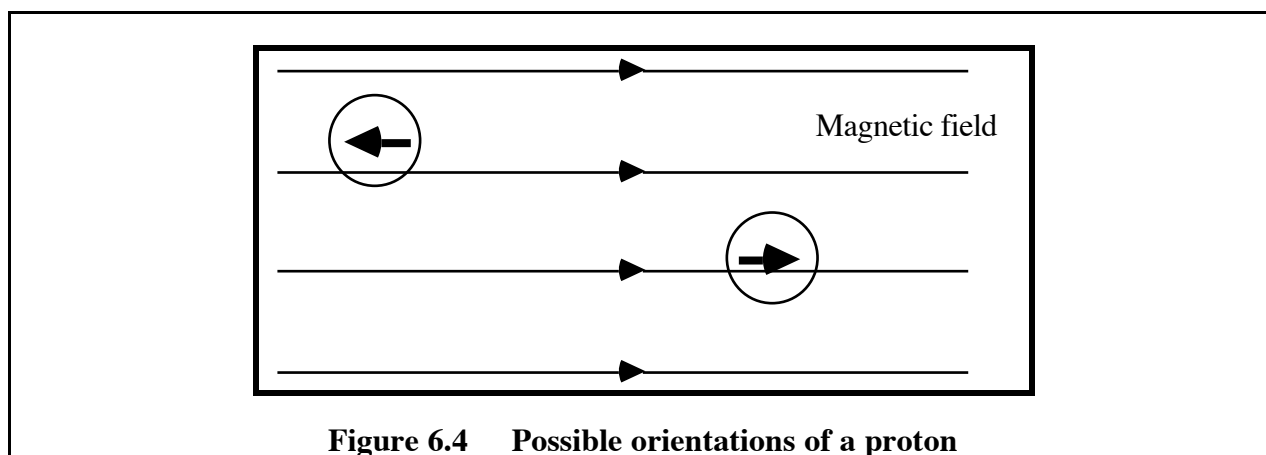


Figure 6.4 Possible orientations of a proton

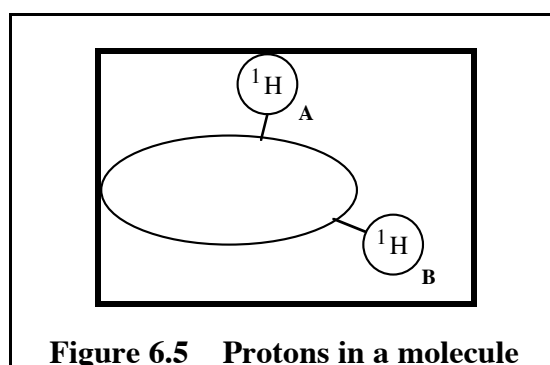
Each orientation has a definite magnetic energy in the field. When photons of energy exactly equal to the energy difference between two orientation states are delivered to the sample, resonance occurs. The atomic nuclei flip between the orientation states resonantly, and in doing so absorb energy from the

incident radiation field. *The energy difference, and hence the resonant frequency, is proportional to the magnetic field strength.*

It turns out that if the sample is placed in a strong magnetic field (of order 1 T) the photons of the requisite energy are in the radio range of frequencies. Most chemicals, and in particular the materials that comprise living animals and plants, are transparent to radio waves, and equally important, are not harmed by them at a low energy densities. So, by placing the creature, plant or sample in an appropriately strong magnetic field, and measuring the absorption of the resonant frequency radio waves, it is possible to measure the amount of hydrogen (^1H) in the sample. Other atoms can be studied similarly, as they have different resonant frequencies in the same magnetic field. It is this basic process which has been refined to such a remarkable degree in NMR.

6-6 NMR SPECTROSCOPY

To understand NMR spectroscopy, consider just two protons in different locations in an organic molecule. The magnetic field at proton A is the vector sum of the externally applied field and the local field of the molecule at point A. In general the local field of the molecule at B will be different. Hence protons A and B are in different total magnetic fields and therefore have different NMR resonant frequencies. So the NMR resonant frequency of each proton in a molecule is different.



Although the magnetic field differences, and hence the energy differences, are small they are readily distinguishable. Frequency is one of the most precisely measurable of all physical quantities. By sweeping the radio frequency through a range (or more usually keeping the frequency constant and sweeping the magnetic field) the resonance of each proton in a molecule is excited in turn. The result is presented as a spectrum which is characteristic of each substance.

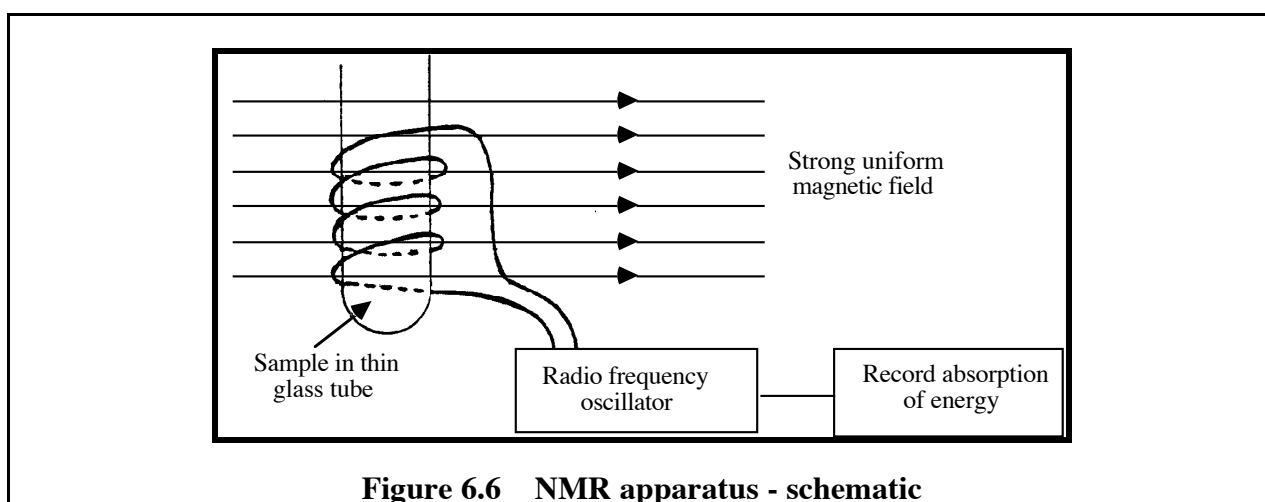


Figure 6.6 does not show the means for sweeping the magnetic field or the oscillator frequency. Nor does it show the separate coil often used for detecting the resonance.

One of the many applications of NMR spectroscopy is in monitoring the progress of biochemical reactions in living things. The upper trace in figure 6.7 is the NMR spectrum of a peptide in living human red blood cells and the lower trace is the NMR spectrum of its hydrolysis products. By watching the spectrum gradually change from one form to the other, it is possible to measure the progress of the reaction in the patient quite harmlessly.

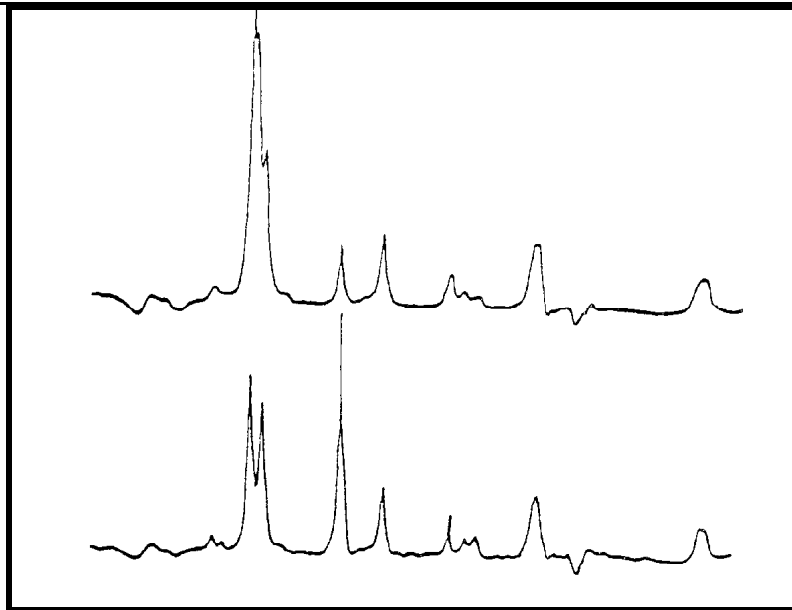


Figure 6.7 NMR spectra
Top: a peptide. Bottom: hydrolysis products.

6-7 NMR IMAGING

In NMR spectroscopy, an important consideration is to make the external magnetic field as uniform as possible throughout the volume of the sample, so that all the molecules are in the same magnetic field and the resulting spectral lines are sharp. By contrast, in **NMR imaging**, the externally applied magnetic field is deliberately made not quite uniform. Then nuclear magnetic resonance occurs only in those regions where the magnetic field strength is exactly the resonance value. The NMR response then measures the total number of protons in that region.

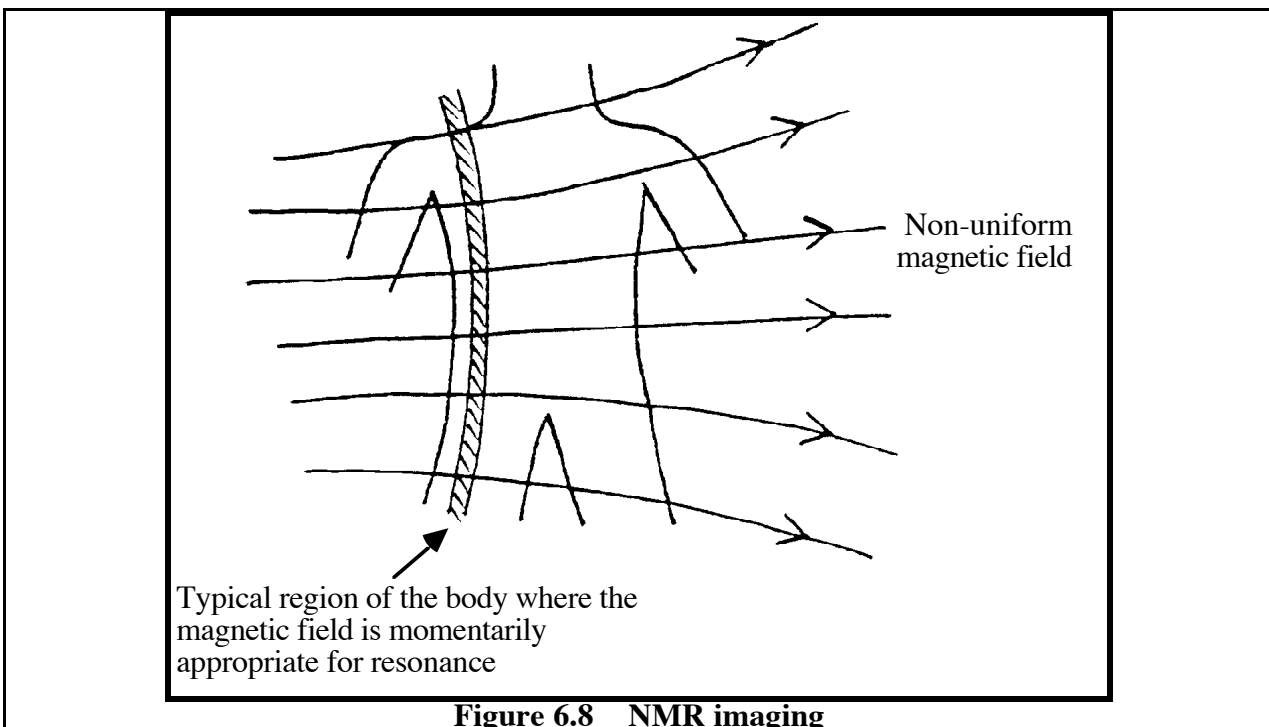


Figure 6.8 NMR imaging

By changing the applied magnetic field, the number of protons in other regions of the patient is measured. By suitably varying the magnetic field, the region of resonance is scanned through the patient, and corresponding measurement of the strength of the resonance is recorded to build up an image of the scanned region. In practice the production of high quality images is achieved by precise computer control of the scanning magnetic field and computer synthesis of the image. The images can be remarkably clear,

and in many soft-tissue examinations these are much better than x-ray images, which are shadows rather than true images.

It is interesting to note that the production of indirect images by computer synthesis was developed initially in radio astronomy; it is physically impossible to build radio telescopes large enough to form real-time images of sufficient resolution. Modern computer technology has made indirect imaging possible in many other disciplines. In medicine **computerised axial tomography** (CAT) and more recently NMR imaging have the potential to go beyond the two-dimensional images of astronomy. In medicine, CAT and NMR techniques can build full three-dimensional images.

QUESTIONS

Q6.1 Find the short wavelength limit for x rays from

- (a) a television tube operated at 10 kV,
- (b) an x ray tube operated at 100 kV,
- (c) a 20 MeV betatron,
- (d) a 1 GeV linear electron accelerator.

Q6.2 From the energy level diagram for molybdenum calculate the approximate energies of the $K\alpha$ and $K\beta$ x-ray photons.

What are the approximate wavelengths of the two x rays? Compare your results with the experimental curves.

What minimum potential difference across an x ray tube is required to excite these x rays? Is this consistent with the experimental curves?