Nuclear Magnetic Resonance

Introduction

Nuclear Magnetic Resonance, or NMR, is a technique used for the spectroscopic analysis of matter. A Swiss physicist named Felix Bloch developed NMR in the 1950s. NMR works by placing the substance in a strong magnetic field that affects the spin of the nuclei. Only a handful of common elements posses the property known as spin, which is essential for NMR to work. A radio wave passing through the substance repositions the nuclei. Once the wave is turned off, the nuclei release energy that contains information about the substance. This information can be translated into an image by using computer techniques.

During the 1980s, NMR was seen as a useful tool for obtaining more precise images of the human body. NMR is accurate and provides doctors with a better idea of what is happening inside someone's body. The images produced are clear and concise, cutting down on the amount of radiation the patient needs to be subjected to. These images are far more accurate than those produced using ultrasonic or CAT scans. NMR is unsurpassed when taking scans of the head and neck. The clarity of images produced has resulted in an increased use of NMR techniques. As a result, NMR is now more commonly referred to as MRI (Magnetic Resonance Imaging), in order to avoid the negative connotations of the word 'Nuclear'. In fact, NMR does not involve any form of radioactivity or ionising radiation. The word 'nuclear' was used to imply the manipulation of small atoms. Subsequently, the medical world has shed the term NMR, and has developed new techniques, which are based on the principles first established by Bloch.

Most matter examined by NMR consists of molecules. Molecules are composed of atoms. For example, a water molecule contains two hydrogen atoms and one oxygen atom. A single hydrogen atom is made up of one proton. This proton possesses a special property known as 'spin'. Spin in an atom can be thought of as a small magnetic field surrounding it. This magnetic field will cause the nucleus to produce the essential NMR signal.

I chose to research into medical physics, as it is a field in which I have little knowledge. Learning things from first principles would give me the opportunity to provide a report from a different perspective. I feel I have been given an opportunity to expand and to learn new ideas, which I wouldn't have been able to do had I chosen a topic, which was familiar to me. Knowing nothing about my chosen topic is like an artist starting work with a blank canvas, as opposed to starting with a half drawn picture.

My aim is to explain the principles behind NMR, and to investigate the underlying physics, which make NMR such a useful tool to the medical world.

Spin Physics

Spin is referred to as angular momentum. There are two types of angular momentum: spin and orbital angular momentum. Spin is a fundamental property of elementary particles. Orbital angular momentum results from the motion of a particle. An electron inside an atom has orbital angular momentum, and spin angular momentum.

The Dutch physicists Samuel Abraham Goudsmit and George Eugene Uhlenbeck first suggested the existence of spin in 1925. Quantum theory was being furiously studied at the time, and the two physicists noticed that certain features of the atomic spectra could not be explained using quantum theory. Not wanting to disprove quantum theory, they added an additional quantum number – the spin of the electron. This allowed the two physicists to give a more complete explanation of atomic spectra.

Spin comes in multiples of ½, and can be either positive or negative. Unpaired electrons, protons, and neutrons each possess a spin of ½. For example, the deuterium atom (^2H), which has one unpaired electron, one unpaired proton, and one unpaired neutron, results in a total electronic spin = ½ and the total nuclear spin = 1. Quantum theory dictates that spin angular momentum can only occur in discrete values.

Nuclei with Spin

Almost every element in the periodic table has an isotope with a non-zero nuclear spin. Here is a list of nuclei routinely used in NMR:

Nuclei	Unpaired Protons	Unpaired Neutrons	Net Spin	γ(MHz/T)
^1H	1	0	1/2	42.58
^2H	1	1	1	6.54
^{31}P	0	1	1/2	17.25
^{23}Na	2	1	3/2	11.27
^{14}N	1	1	1	3.08
^{13}C	0	1	1/2	10.71
^{19}F	0	1	1/2	40.08

When placed in a magnetic field of strength B, a particle with spin can absorb a photon of frequency *f*. The frequency *f* depends on the gyromagnetic ratio, γ of the particle. So $f = \gamma B$

For hydrogen, γ = 42.58 MHz / T.

Energy Levels

To understand how particles with spin behave in a magnetic field, consider a proton. The proton has a property called spin. The spin can be looked at as being a magnetic moment vector, which causes the proton to behave like a magnet with a north and south pole. When this proton is placed into a magnetic field, the spin vector aligns itself with the field. A magnet would do the same. There are low and high-energy states. The low energy configuration is where the poles are aligned at N-S-N-S. The high-energy configuration is when the poles are aligned N-N-S-S.

This particle can go through a transition between the two energy levels by the absorption of a photon. A particle in the low energy configuration would have to absorb a photon to end up in the high-energy state. However, the energy of this photon must exactly match the difference between the two energy levels. The energy of a photon is related by its frequency by Planck's constant ($h = 6.6 \times 10^{-34}$ J s)

$$E = h f$$

We have seen that $f = \gamma B$ and $E = h f$, therefore, if we equate the two formulae, we get a single formula that gives us the energy of the photon needed to cause a transition between energy levels.

$E = h f$

$f = \gamma B$

$\therefore \quad E = h \gamma B$

When the energy of a photon exactly matches the energy difference between the two spin states, an absorption of energy occurs.

NMR Hardware

Hardware Overview

Once the material has been placed into a magnetic field, it gives off an NMR signal. This signal is useless without the correct hardware to translate and display the information.

The graphics window displays a schematic of the major systems of a nuclear magnetic resonance spectrometer, and a few of the major interconnections. The superconducting magnet of the NMR spectrometer is found near the top of the schematic. The magnet produces the B_0 magnetic field necessary. Within the bore of the magnet are the shim coils for homogenizing the B_0 field. Within the shim coils is the probe. The probe contains the RF coils necessary for producing the B_1 field, which is used to rotate the spins by 90° or 180°.

The heart of the spectrometer is the computer. It regulates each of the components in the spectrometer. The RF components under the control of the computer are the RF frequency source and pulse programmer. The source is used to generate a sinusoidal wave of the desired frequency. The pulse programmer is used to set the width of the RF pulses. An RF amplifier is used to increase the pulses power from milli-Watts to tens or hundreds of Watts. The computer is also used to control the gradient pulse programmer, which sets the shape and amplitude of gradient fields. A gradient amplifier is used to increase the power of the gradient pulses.

The human operator of the spectrometer gives input to the computer via a separate console terminal with a keyboard and mouse. Pulse sequences are selected and customized through the console terminal. The operator is able to see the spectra on the video display located on the console. Hard copies of the display can be made via a printer.

Magnet

The NMR magnet is possibly the most expensive component of the nuclear magnetic resonance spectrometer system. It is a superconducting magnet. A superconducting magnet has an electromagnet made of superconducting wire. Superconducting wire has a resistance near to zero when it is cooled to a temperature of –273.15°C or 0 K. This is absolute zero, and is obtained by keeping the wire in liquid helium. The length of the superconducting wire is typically several miles long. The wire is wound into a multi-turn solenoid. The coil of wire is kept in liquid helium. The liquid helium and wire are kept in a small chamber, which in turn is kept at a constant temperature of 77.4 K. This acts as a thermal buffer between the room temperature air and the liquid helium.

Carbon – 13 NMR

Most of the molecules studied by NMR contain carbon. Unfortunately, carbon-12 does not have a nuclear spin, but carbon-13 does. This is due to the presence of an unpaired neutron. Carbon-13 makes up approximately 1% of the carbon nuclei on Earth. Therefore, carbon-13 spectroscopy will be less sensitive than hydrogen NMR spectroscopy.

Advancements in superconducting magnet design and RF sample coil efficiency have helped to make carbon-13 spectroscopy routine on most NMR experiments.

Evaluation

The research was extremely enlightening. The usefulness of NMR has been highlighted to me, and I have applied my knowledge of physics to the various processes. The AS-Physics textbook gave a general overview of what NMR was, and how it worked on an atomic level. Although these descriptions were sufficient, they failed to emphasize key areas and formulae. The Longmans A-Level Physics textbook gave an insight into spin physics. The textbook gave a simple model for the spin of atoms, as well as providing a small mention of quantum theory, and how the existence of spin was discovered. Microsoft Encarta 1997 showed similar levels of detail on NMR and spin physics. The CD also gave a detailed breakdown of what spin physics entails and how it applies to NMR. The CD concentrated more on analogies and visualisations to help the understanding of the concepts, while the textbook preferred to underline the relevant physics. The images are provided by the CD. Perhaps the most helpful of the sources was a website written by Professor Joseph P. Hornak. His website outlined the specific hardware requirements and how the physics is applied to them. His descriptions of spin physics were also very visual. Although much of the material was beyond my understanding, reading the other textbooks and looking up key terms, allowed me to grasp the basic ideas being described.

Bibliography

Author	Name of source	Pages used
Microsoft	Microsoft Encarta 97	*NMR, MRI, spin physics, history of NMR, various historic references*
Joseph P. Hornak Ph.D.	NMR-MAIN http://www.rochester.uc.com/chem/nmr/nmrmain.html	*Spin physics, NMR Hardware*
Jim Breithaupt & Ken Dunn	Letts A-Level Physics	*Basic formulae, key terms reference*
Longmans	Longmans A-Level Study Guide	*Quantum theory, spin physics*

Journal

- Establish topic
- Primary research involving learning of first principles and relevant physics involved in advanced concepts
- Secondary research involving uses of NMR and various historic reference points
- Begin writing project, referring to sources when needed
- Compare and contrast information on spin physics
- Begin research into hardware used
- Evaluate sources and finish writing project