

5.2: The Origin of the NMR Signal

The Magnetic Moment

Nuclear magnetic resonance spectroscopy is an incredibly powerful tool for organic chemists because it allows us to analyze the connectivity of carbon and hydrogen atoms in molecules. The basis for NMR is the observation that many atomic nuclei generate their own magnetic field, or magnetic moment, as they spin about their axes. Not all nuclei have a magnetic moment. Fortunately for organic chemists, though, hydrogen (^1H), the ^{13}C isotope of carbon, the ^{19}F isotope of fluorine, and the ^{31}P isotope of phosphorus all have magnetic moments and therefore can be observed by NMR – they are, in other words, NMR-active. Other nuclei – such as the common ^{12}C and ^{16}O isotopes of carbon and oxygen – do not have magnetic moments, and cannot be directly observed by NMR. Still other nuclei such as the hydrogen isotope deuterium (^2H) and nitrogen (^{14}N) have magnetic moments and are NMR-active, but the nature of their magnetic moments is such that analysis of these nuclei by NMR is more complex.

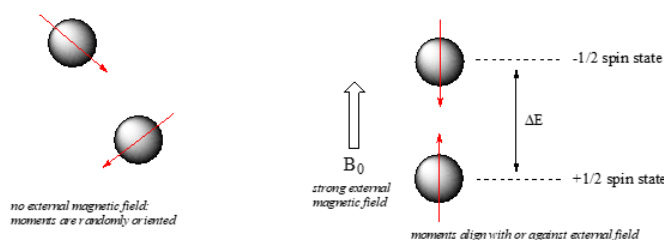
In practice it is ^1H and ^{13}C nuclei that are most commonly observed by NMR spectroscopy, and it is on those techniques that we will focus in this chapter, beginning with ^1H -NMR. The terms ‘proton’ and ‘hydrogen’ are used interchangeably when discussing because the ^1H nucleus is just a single proton.

Table 5.2.1 : Some examples of magnetic and nonmagnetic nuclei relevant to biological organic chemistry.

Magnetic Nuclei	Nonmagnetic Nuclei
^1H	^{12}C
^2H	^{16}O
^{13}C	^{32}S
^{14}N	
^{19}F	
^{31}P	

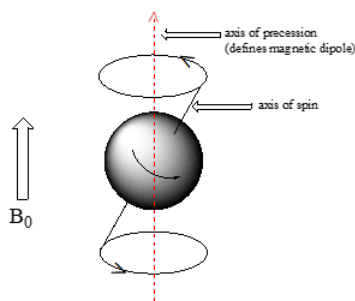
Spin States and the Magnetic Transition

When a sample of an organic compound is sitting in a flask on a laboratory bench, the magnetic moments of all of its protons are randomly oriented. However, when the same sample is placed within the field of a very strong superconducting magnet (this field is referred to by NMR spectroscopists as the applied field, abbreviated B_0) each proton will assume one of two possible quantum spin states. In the $+\frac{1}{2}$ spin state, the proton's magnetic moment is aligned with the direction of B_0 , while in the $-\frac{1}{2}$ spin state it is aligned opposed to the direction of B_0 .



$+\frac{1}{2}$ spin state is slightly lower in energy than the $-\frac{1}{2}$ state, and the energy gap between them, which we will call ΔE , depends upon the strength of B_0 : a stronger applied field results in a larger ΔE . For a large population of organic molecules in an applied field, slightly more than half of the protons will occupy the lower energy $+\frac{1}{2}$ spin state, while slightly less than half will occupy the higher energy $-\frac{1}{2}$ spin state. It is this population difference (between the two spin states) that is exploited by NMR, and the difference increases with the strength of the applied magnetic field.

At this point, we need to look a little more closely at how a proton spins in an applied magnetic field. You may recall playing with spinning tops as a child. When a top slows down a little and the spin axis is no longer completely vertical, it begins to exhibit precessional motion, as the spin axis rotates slowly around the vertical. In the same way, hydrogen atoms spinning in an applied magnetic field also exhibit precessional motion about a vertical axis. It is this axis (which is either parallel or antiparallel to B_0) that defines the proton's magnetic moment.

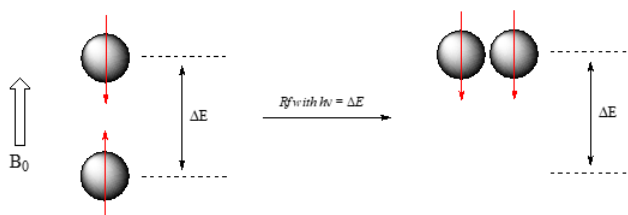


Watch the first minute or so of this [video of spinning tops](#): look for the precessional motion

The frequency of precession (also called the Larmour frequency, abbreviated ν_L) is simply the number of times per second that the proton precesses in a complete circle. A proton's precessional frequency increases with the strength of B_0 .

If a proton that is precessing in an applied magnetic field is exposed to electromagnetic radiation of a frequency ν that matches its precessional frequency ν_L , we have a condition called resonance. In the resonance condition, a proton in the lower-energy $+\frac{1}{2}$ spin state (aligned with B_0) will transition (flip) to the higher energy $-\frac{1}{2}$ spin state (opposed to B_0). In doing so, it will absorb radiation at this resonance frequency ν - and this frequency corresponds to ΔE ,

the energy difference between the proton's two spin states. With the strong magnetic fields generated by the superconducting magnets used in modern NMR instruments, the resonance frequency for protons falls within the radio-wave range, anywhere from 100 MHz to 800 MHz depending on the strength of the magnet.



Think back for a moment to the other two spectroscopic techniques we have learned about: IR and UV-Vis spectroscopy. Recall from section 4.2 that photons of electromagnetic radiation of a given frequency correspond to energy (E) given by $E = h\nu$, where h is Planck's constant and ν is the frequency in waves per second, or Hz. Recall also from section 4.3 that the energy gap between vibrational states corresponds to the energy associated with infrared radiation, and from section 4.4 that the energy gap between electronic states in conjugated p-bonding systems corresponds to the energy associated with light in the ultraviolet and visible regions of the electromagnetic spectrum. Now, we know that in NMR, the energy gap ΔE between the $+\frac{1}{2}$ and $-\frac{1}{2}$ spin states of an atomic nucleus in a strong magnetic field corresponds to the energy associated with radiation in the radio frequency (Rf) region of the spectrum.

By detecting the frequency of Rf radiation that is absorbed, we can gain information about the chemical environment of protons in an organic molecule.

? Exercise 5.2.1

In a general sense, how big is the energy gap for the nuclear spin transition observed in NMR compared to the energy gap for the vibrational transition observed in IR spectroscopy? Much bigger? Much smaller? Slightly bigger or smaller? About the same? How can you tell from the information presented in this section?

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