§9.1.1 General Principles

1. Nuclear Spi

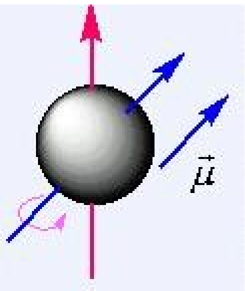
Spinning of unpaired electrons at the nuclear makes the magnetic momentum:

Spin angular momentum as:

$$\rho = \frac{h}{2\pi}\sqrt{I(I+1)}$$

The magnetic momentum can be calculated as:

$$\mu = g\beta\sqrt{I(I+1)}$$



I is the spin quantum number,

h is the plank constant

the nuclear magneton $\beta = eh/2Mc$;

If I does not equal to zero, the magnetic momentum should be observable.

The spin at the nuclear is normally expressed by I :

Mass Number	Atomic Number	Spin Quantum Number (I)
Even	Even	0
Even	Odd	1,2,3
Odd	Odd or Even	1/2, 3/2, 5/2,

Discussion:

(1). For those nuclei with I equals to 0, such as O(16), C(12), S(22) and etc, there is no unpaired electrons at the nuclei, so

there is not resonance adsorption and the magnetic momentum is not observable.

- (2). For those nuclei with I equals to 1 or are larger than 0, such as

  I=1: ^{12}H, ^{14}N ;

  I=3/2: ^{11}B, ^{35}Cl, ^{79}Br, ^{81}Br;

  I=5/2: ^{17}O, ^{127}I .

As these nuclei have 3 or more possible spin states in a magnetic field, their resonance adsorption are more complex, and their application are

constrained.

- (3) I = 1/2: ^{1}H, ^{13}C, ^{19}F, ^{31}P

For those nuclei with I equals to 1/2. The charge is finely distributed as a sphere. It will rotate like a top, and create magnetic moments. For .

their simplicity, they are well studied. Also, C and H are main component elements for organic compounds. The nuclear resonance spectrum of

1H is called H-NMR, and is used widely. The nuclear resonance spectrum of 13C is normally called C-NMR. H-NMR is mainly discussed in this

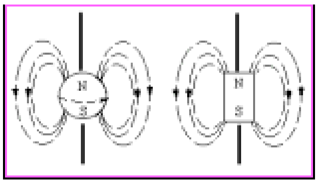
chapter

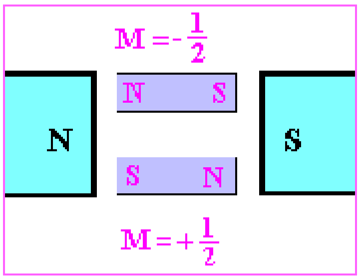
2.Nuclear Magnetic Resonance

For nuclei with spin quantum equals to 1/2 (such as hydrogen), the charge is finely distributed as a sphere. They will spin as a top and

create a small magnetic field.

When it is placed in an external magnetic field, there is 2I+1 orientations compared to the external field.





For ^{1}H nuclei (I=1/2), there are 2 orientations (2 energy levels)

(1). Low energy level, which is parallel to the external magnetic field, the magnetic quantum number is +1/2

(2). High energy level, which is reverse to the external magnetic field, and the magnetic quantum number is —1/2.

For these 2 orientations, they are not completely parallel to the external field. The intersection angles are 54°24' and 125°36' respectively.

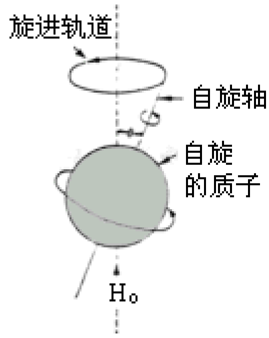
The overall interaction of these magnetic field results in production of Larmor precession. The precession frequency $\nu 0$, and angular velocity ω

have the following relationship:

$$\omega_0 = 2\pi\nu_0 = \gamma H_0$$

Where γ is the magnetogyric ratio and H0 is the external magnetic field. The energy level difference between these 2 orientations can be expressed as:

$\triangle E = \mu H0$



3. Requirements for NMR

In existance of an external magnetic field, the energy level of nuclei splits. When excitation

from lower energy level to higher energy level occurs, energy is needed as theenergy level

is quantized.

Electromagnet products electromagnetic wave, provides the energy for NMR.

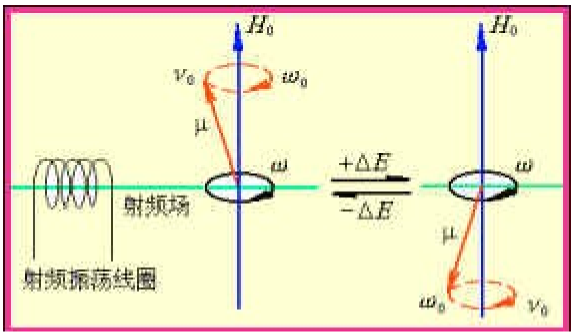
For ^{1}H nuclei, the energy level difference is : $\triangle E = \mu H_0$

The energy required for NMR to occur is:$\triangle E = \mu H_0 = h\nu_0$

According to Larmor precession equation:$\omega_0 = 2\pi\nu_0 = \gamma H_0$

The requirements for NMR is:

$\nu_0 = \gamma H_0/(2\pi)$



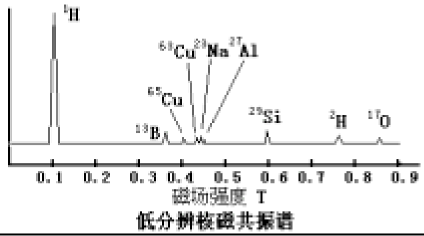
- (1). Unpaired electrons
- (2). External magnetic field, and split of energy level;

(3). Radiation frequency and the strength of the external force field satisfies the following relation:

$$\nu_0 / H_0 = \gamma / (2\pi)$$

Discussion:

According to requirements for NMR to occur:



$$\nu_0 \ / \ H_0 = \gamma / (2\pi)$$

(1).For the same nuclei, magnetogyric ratio γ is definite, if external magnetic field varies, the frequency υ

- changes.

(2).For different nuclei, magnetogyric ratio γ is different, therefore, the requirements for NMR to occur is different, especially intensity of external magnetic field and the frequency.

- (3).Keep the magnetic field intensity as a constant; varying the frequency, NMR will occur at different

frequencies. As an alternative, the frequency can be kept as a constant, and varying the intensity of the external magnetic field, NMR will also occur at different intensity.

For 1H:

Intensity of the external magnetic field	Resonance frequency
1.409 T	60.0 MHz
2.305 T	100.0 MHz

Unit of intensity of external force field is GS, 1GS equals to 10-4 T.

In 1950, Proctor et al. found that H-NMR is in relation with its structure (chemical environment). At high resolution, adsorption peaks shift and split.