335(1): Modification to the Spin Spin NMR Hamiltonian

Consider the interaction between the spin of the electron and the spin of the proton in a molecule. The simplest example is atomic hydrogen, H, in which there is an electron and one proton. The nucleus of H consists of one proton. The spin Hamiltonian of the nucleus is:

$$H_N = -g_N \frac{e}{2m_p} \underset{\sim}{I} \cdot \underline{B} \quad -(1)$$

where for ^1H:

$$\underline{I} = 1/2, \quad g_N = 5.5857 \quad -(2)$$

Here m_p is the mass of the proton, and $\underset{\sim}{I}$ is the nuclear spin angular momentum. Eq. (1) is the basis for proton nuclear magnetic resonance (NMR).

If the magnetic flux density of the spectrometer is aligned in the Z axis:

$$H_N = -g_N \frac{e}{2m_p} I_Z B_Z \quad -(3)$$

where

$$I_Z \psi = \hbar m_I \psi \quad -(4)$$

and

$$m_I = -\underline{I}, \dots, \underline{I}. \quad -(5)$$

In this case the energy of interaction is:

2)

$$E = \langle H_N \rangle = -g_N \frac{e\hbar}{2m_p} m_I B_Z \quad -(6)$$

where

$$m_I = \pm 1/2 \quad -(7)$$

for the proton in a nucleus. For absorption of radiation:

$$\Delta m_I = 1 \quad -(8)$$

so

$$\hbar\omega_{res} = E(m_L = -1/2) - E(m_L = 1/2)$$

$$= g_N \frac{e\hbar}{2m_p} B_Z \quad -(9)$$

at the NMR resonance frequency ω_{res}. So

$$\boxed{\omega_{res} = g_N \frac{e}{2m_p} B_Z} \quad -(10)$$

In the presence of the electron, the complete spin hamiltonian is: $-(11)$

$$\boxed{H = -\frac{e}{m_e} \underline{S} \cdot \underline{B} - g_N \frac{e}{2m_p} \underline{I} \cdot \underline{B}}$$

in which the electron spin hamiltonian:

$$H_S = -\frac{e}{m_e} \underline{S} \cdot \underline{B} \quad -(12)$$

originates in the Dirac equation and use of the Dirac approximation. The rigorous solution of the classical hamiltonian gives:

$$H_S = - 2\frac{e}{m_e} \left(\frac{\gamma^2}{1+\gamma} \right) \underline{S} \cdot \underline{B} \quad -(13)$$

as in Note 334(3). So the spin-spin hamiltonian (11) is modified to:

$$H = - 2\frac{e}{m_e} \left(\frac{\gamma^2}{1+\gamma} \right) \underline{S} \cdot \underline{B} - g_N \frac{e}{2m_p} \underset{\sim}{I} \cdot \underline{B} \quad -(14)$$

So the corrections in the type one hamiltonian have an effect on nuclear magnetic resonance.

The hamiltonian (14) is developed in the next note.