CHEM 352: Examples for chapter 7.

1. What is the resonance frequency for ^{19}F at 1 T field? The value for g_N for this nucleus is 5.256.

Solution:

The resonance condition is:

$$\Delta E = g_N \mu_N B = (5.256) \times (5.051 \times 10^{-27}\ \text{J/T})(1\ \text{T}) = 2.655 \times 10^{-26}\ \text{J}$$

This can be converted to resonance frequency (ν) according to:

$$\nu = \frac{\Delta E}{h} = \frac{2.655 \times 10^{-26}\ \text{J}}{6.626 \times 10^{-34}\ \text{Js}} = 40.07\ \text{MHz}$$

---

2. Proton has a nuclear spin of 1/2, which means that the degenerate nulcear spin states split into two separate states in the presence of external magnetic field. What is the difference between spin populations in the lower vs. upper nuclear spin states for protons at 1 T field and room temperature? The g_N value for proton is 5.585. Normalize your answer with respect to the total spin population.

Solution:

The spin populations (N_α and N_β) follow the Boltzmann law (see thermodynamics notes). Since we are at relatively high temperature, we can approximate the exponential function as $e^x \approx 1 + x$ (first two terms of the Taylor series).

$$\frac{N_\alpha}{N_\beta} = 1 + \frac{g_N \mu_N B}{kT} = 1 + \frac{(5.585)(5.05 \times 10^{-27}\ \text{J/T})(1\ \text{T})}{(1.38 \times 10^{-23}\ \text{J/K})(298\ \text{K})} = 1 + 6.86 \times 10^{-6}$$

Based on this we have then the difference between the two spin states (normalized by the total number of spins) is:

$$\frac{N_\alpha - N_\beta}{N_\alpha + N_\beta} = 3.43 \times 10^{-6}$$

(solve for N_α in terms of N_β in the first equation and plug into the second)

3. What is the magnitude of magnetic field that is required for a free electron to have a resonance frequency of 9.500 GHz. For free electron $g_e \approx 2.0023$.

Solution:

Based on the electron spin resonance condition we can get:

$$B = \frac{h\nu}{g_e \mu_B} = \frac{(6.6262 \times 10^{-34}\ \text{Js})(9.500 \times 10^9\ \text{s}^{-1})}{(2.0023)(9.2741 \times 10^{-24}\ \text{Am}^2)} = 0.3390\ \text{T} = 3390\ \text{Gauss}$$

4. When frozen blood sample is measured with Electron Spin Resonance spectrometer (9.41756 GHz) shows a broad peak at 1629.0 Gauss. What is the g-value for this peak?

Solution:

From the resonance condition for this line is we get:

$$g = \frac{h\nu}{\mu_B B_0} = \frac{(6.6262 \times 10^{-34}\ \text{Js})(9.41756 \times 10^9\ \text{s}^{-1})}{(9.27408 \times 10^{-24}\ \text{Am}^2)(0.16290\ \text{T})} = 4.1308$$

Based on this value, this is likely Fe^{3+} complex (open shell). This could be, for example, from methemoglobin.