

Calculating the energy levels of spin states:

The energy difference between the spin states of a nucleus in a magnetic field can be easily calculated if the frequency of the NMR signal is known by using the formula: $E = h\nu$ where h is Planck's constant $6.6 \times 10^{-34} \text{ J}\cdot\text{s}$ and ν is the frequency in Hz.

Thus, the energy separation of the two spin states of H in the EFT instrument is:

$$E = (6.6 \times 10^{-34} \text{ J}\cdot\text{s})(60 \times 10^6 \text{ s}^{-1}) = 3.96 \times 10^{-26} \text{ J},$$

which is equivalent to 0.0238 J/mol

This energy is very small compared to visible light or common chemical energies both of which are in the range of $3 \times 10^{-19} \text{ J/molecule}$ or 200 kJ/mol (i.e. *ca.* 10 million times larger). The energy of the spin states is even much smaller than ambient temperature thermal energy of about 2400 J/mol and so the population differences between the two spin states will be small. This has practical implications that will be discussed in class.

Spin states of nuclei with I not equal to 1/2.

The spin states that a nuclei can take will be all values between $-I$ and $+I$ in steps of 1. For nuclei such as C-13, H-1, N-15, F-19, and P-31 that have $I = 1/2$ there are just two spin states of $-1/2$ and $+1/2$.

Some nuclei have spins of greater than $1/2$ such as H-2 that has a spin number of 1 so it can take three orientations in a magnetic field corresponding to spin states of $-1, 0, +1$ or 3 different spins. This appears commonly in the C-13 spectra of solvents that are have deuterium or heavy hydrogen in them. The carbons attached to the H-2 will be coupled to it and if H-2 is present it will show up as a 1:1:1 triplet; if 2 H-2 are attached to the C-13, the C-13 peak will show up as a 1:2:3:2:1 pentet.

Signal-to-noise ratios

The signal to noise values can be calculated manually by 1) measuring the height of peak, HS , (the distance from the top of the peak to the middle of the baseline noise), 2) measuring the peak-to-peak height of the noise, HN (the total distance that includes all of the noise), or 3) calculating the average noise, AV , by dividing the peak-to-peak noise by 2.5 ($AV = HN/2.5$). The S/N ratio is then calculated as (HS/AV) .

Principles Lab – High/Low Field instruments - 2. Carbon-13.

Collect a C-13 spectrum of ethyl benzene on the Avance III 400. For all spectra, use $ns=16$. **After the spectrum is obtained on the Avance III; use the “dsn” command to have the computer calculate the signal-to-noise ratio for your spectrum and you should write it down on the plot.** Identify all peaks including any reference compound or solvent peaks.

Then calculate the signal-to-noise ratio manually. Show your calculations. Does your calculated value agree approximately with the computer-calculated value? Briefly comment on the S/N ratio. (e.g. How well does your value compare with the instrument calculated value and why might they be different if you believe the difference is significant? How clear are the peaks from the noise and at what point do you think the S/N ratio would tell you that a “peak” was not really something from your sample?)