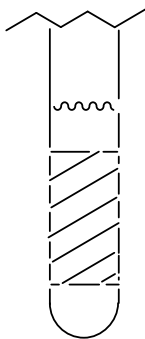


NMR SPECTROSCOPY – In-class Questions – Set 1 – Basic Concepts

1. What makes up the nucleus of a hydrogen atom?
2. What are the allowable spin quantum numbers for an electron?
3. What do you think are the allowable spin quantum numbers for a proton?
4. What is the magnitude of I , the total nuclear spin, for a hydrogen nucleus?
5. What do you think is produced by the spinning, charged proton that is the hydrogen nucleus?
6. What happens when two magnetic fields (B_p and B_{APPL}) are in contact with each other?
7. What do you think are the two allowable orientations of B_p relative to B_{APPL} ?
8. Do you think the two allowable orientations have the same or different energy?
9. Which of the two do you think is lower in energy?

NMR SPECTROSCOPY – In-class Questions – Set 2 – Energy Transition and Population

1. What frequency of electromagnetic radiation is needed to excite a nuclear spin flip?
2. Where is radiofrequency (RF) radiation on the energy scale of the electromagnetic spectrum?
3. Is the thermal energy at room temperature large or small compared to the energy of a π - π^* transition and to the energy of a nuclear spin flip? What are the consequences of your answers to these questions?
4. If thermal energy has sufficient energy to excite nuclear spin flips, why are there still more in the ground than excited state?
5. Can you think of two processes by which a specific excited state nucleus can get rid of its excess energy?
6. Do excited state nuclei have short or long relaxation times?
7. When the populations of the two levels are equal, can we continue to excite ground state nuclei up to the excited state such that the population of the excited state becomes larger than the population of the ground state, creating what is known as a population inversion?
8. What happens to the population distribution as the energy gap between the ground and excited state is increased?
9. Consider a sample in an NMR tube. The crosshatched region in the tube is the area over which signal is recorded. Why is it important that B_{APPL} be homogeneous over this entire region?

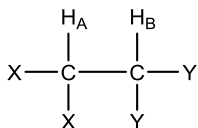


NMR SPECTROSCOPY – In-class Questions – Set 3 – Electron Shielding

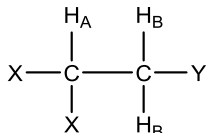
1. What “things” in a molecule generate magnetic fields that will influence B_0 for a particular hydrogen nucleus?
2. Does electron density affect the magnitude of B_e ? If so, what is the relationship?
3. Does a more highly shielded nucleus absorb higher frequency (higher energy) or lower frequency (lower energy) radiation?
4. Suppose the resonant frequency of the TMS singlet on a 400 MHz NMR spectrometer is exactly 400 MHz. What is the chemical shift in ppm for a signal that has a resonant frequency of 400,000,400 Hz?
5. What is different as B_{APPL} is varied?

NMR SPECTROSCOPY – In-class Questions – Set 4– Nuclear Coupling

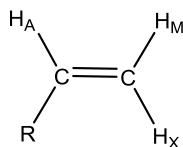
1. Consider the two hydrogen atoms H_A and H_B in the compound shown below. The X and Y groups are not hydrogen atoms and produce no magnetic fields. In particular, let's focus on the effect that H_B has on H_A . We can think of H_A "looking over" at H_B and ask ourselves about the magnetic field produced by H_B .



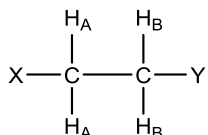
2. What do you know from earlier in this unit about the magnetic field produced by H_B ?
3. Is the flip of H_B 's spin between the "with" and "against" states rapid or slow?
4. What does the resonance for H_A look like in the NMR spectrum?
5. Which peak in the doublet corresponds to B_{HB} "with" and which corresponds to B_{HB} "against"?
6. Can you think of a way to decouple a hydrogen atom like H_B ?
7. What would the H_B resonance look like?
8. What would the resonance for H_A look like in the compound shown below where there are two H_B protons? Provide a rationale for your answer.



9. Which peak of the triplet corresponds to the WW and which to the AA situation?
10. What factors do you think influence the magnitude of the coupling constant?
11. Predict the coupling constants that would occur between H_A , H_M and H_X and the mono-substituted alkene shown below and draw the shape of each resonance.

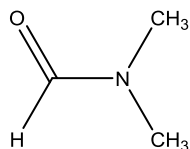


12. Consider the following compound in which $J_{AB} = 10$ Hz, $\delta_{H_A} = 1.3$ ppm and $\delta_{H_B} = 1.2$ ppm. Draw the resulting spectrum if the spectrum is recorded on a 100 MHz and 400 MHz spectrometer.

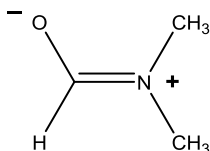


NMR SPECTROSCOPY – In-class Questions – Set 5 – Exchange Effects

1. Considering the spectrum of a compound such as methanol (CH_3OH). Using the rules for coupling we have established, predict the number of resonances and identify their multiplet structure.
2. However, in other situations the spectrum of methanol appears as two singlets, one of area three and the other of area one. Propose a reason why singlets are observed instead of coupled multiplets.
3. Another time-dependent aspect to consider about NMR spectra can be illustrated by considering the ^1H NMR spectrum of *N,N*-dimethylacetamide (DMA) shown below.



4. What does the NMR spectrum of DMA look like?
5. DMA has the following contributing resonance form. What would the NMR spectrum of DMA look like in this resonance form?



NMR SPECTROSCOPY – In-class Questions – Set 6 – Classical Description

1. What happens when an electrical current is run through a wire coil?
2. What happens to the nucleus after B_1 is turned off?
3. Suppose a wire coil is placed on the Y-axis. What happens in the wire coil as the magnetic field of the tipped nucleus is imparted on it?
4. Draw the current profile that would result in the wire coil on the X-axis as the tipped nucleus relaxes back to its ground state.
5. Draw the FID that would result if the nucleus had a much shorter relaxation time.
6. Do you see a problem with performing a FT on an FID with a very short relaxation time? If so, what would happen in the resulting frequency domain spectrum?
7. Where is the amplitude of peaks determined in the FID?
8. Why is a delay time incorporated into the sequence?
9. Why are the advantages and disadvantages of using 30° pulses instead of 90° pulses?
10. What is the advantage of recording several FIDs and adding them together?
11. Suppose the following pulse sequence is used to obtain the spectrum of a ^{13}C nucleus with a spin-lattice relaxation time of 100 seconds (90° pulse, 1 second collection of the FID, 1 second delay). Note, carbon atoms with no directly bonded hydrogen atoms can have relaxation times as long as 100 seconds. This pulse sequence is repeated four times.
 - Draw the position of the ^{13}C magnetization vector after each of the four pulses.
 - Draw the corresponding FID that would be obtained after each pulse.
 - Draw the composite FID obtained by adding the four individual FIDs together.
 - What do you observe for this carbon in the resulting frequency domain spectrum?