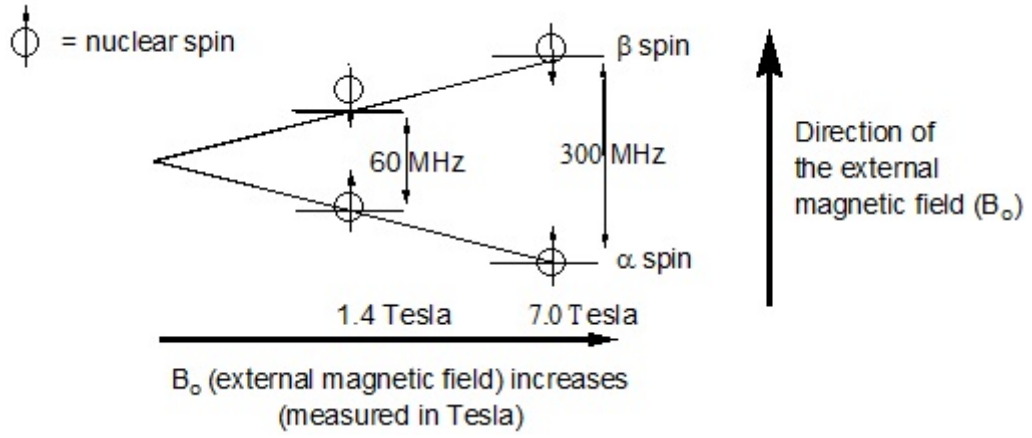
Name:_____

Nuclear Magnetic Resonance (NMR) Theory

Model 1: Effect of External Magnetic Field on Energy



1. Based on the direction of the external magnetic field, what is the orientation of the spin of nuclei having an alpha (α) spin state? Of nuclei with a beta (β) spin state?

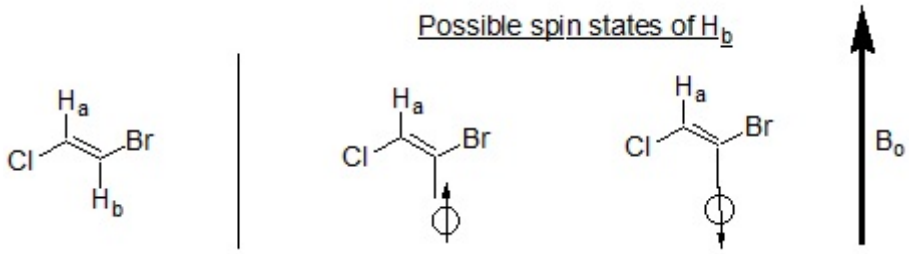
2. Which is more stable, nuclei having an α spin or nuclei with a β spin?

3. What happens to the difference in energy between alpha and beta spin states as the strength of the external magnetic field (B_o) increases?

4. Is the external magnetic field (B_o) directly or inversely proportional to the ΔE between the two spin states?

5. What region of the electromagnetic spectrum correlates to the difference in energy (ΔE) between alpha and beta spin states? (You may need to refer to Ch. 12 or 13 in your book).

Model 2: Spin-Spin Splitting (Coupling) Basics



6. What are the possible spin states of H_b in the model above?

7. Nuclei within 2 to 3 bonds of each other and in different chemical environments slightly alter each others chemical shift based on the direction of their nuclear spin. If H_b has an alpha spin state, will the effective magnetic field experienced by H_a increase, decrease or remain the same?

8. How will this effect ΔE between the alpha and beta spin states of H_a?

9. If H_b has a beta spin state, how will ΔE between the alpha and beta spin states of H_a be effected?

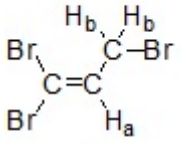
10. How many peaks are needed to represent H_a in the ^1H NMR spectrum of this compound?

11. How many peaks are needed to represent H_b in the ^1H NMR spectrum of this compound?

12. Do you think the gap between peaks representing H_a would be the same or different then the gap between peaks representing H_b? Explain.

Note: If two hydrogens split each other they do so to the same extent. The gap between peaks is referred to as a coupling constant (J value).

Model 3: Spin-spin splitting application



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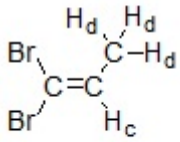
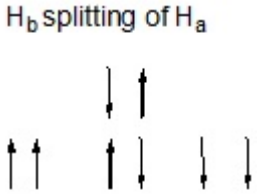


2



13. Based on model 2, how will H_b be split by H_a in model 3?

14. According to the spin-spin splitting diagram of H_a by H_b in structure 1:

    a. How many peaks would be needed to represent H_a in this ^1H NMR spectrum?

    b. What is the expected ratio of area for each of those peaks?

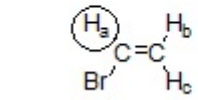
    c. Should the total width (in Hz) of the splitting pattern of H_a be half as much, the same, or twice as much as the splitting pattern for H_b? Justify your answer.

15. Use the spin-spin splitting diagram depicted for H_a above to provide a diagram for the splitting of H_c by H_d. Use the space next to the structure above.

    a. How many peaks will represent H_c? What is the ratio of those peaks in the splitting pattern?

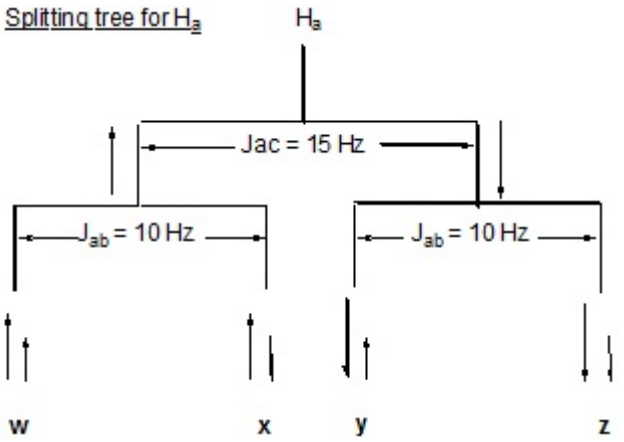
16. If N is equal to the number of protons in an environment, provide an equation that can be used to predict the number of peaks created by that proton environment

Model #4: Complex Splitting



H_a split by H_c: J_{ac} = 15 Hz

H_a split by H_b: J_{ab} = 10 Hz



17. How many different proton environments are there in the structure above?

Note: Protons that are either nearly parallel or anti-parallel generally have large J values. Protons that are nearly perpendicular have small J values.

18. Based on the statement above and the given coupling constants, what is your prediction of the value of J_{bc}? Explain.

19. What is the distance (in Hz) between **w** and **z** (total width of splitting pattern) in the splitting tree above?

20. The coupling constant J_{ab} is represented by the gap between **w** and **x** or **y** and **z**. The gap between which letters correlates to the value of J_{ac}?

21. The splitting pattern above is called a doublet of doublets (dd). What is the ratio of area for each peak in this splitting pattern?

22. Name two ways in which this splitting pattern differs from a quartet.

23. If the Jbc coupling constant is 1 Hz, provide a splitting tree similar to the one above for H_b. Hint: Begin with the largest coupling first.