

Objectives for Chapter 5 – NMR

I. Introduction to NMR

1. Give a brief description of NMR, including what peaks represent, and what you can learn about a compound.
2. State what property causes atoms to be detected by NMR, and what isotopes are commonly used in NMR.
3. Describe what an NMR spectrum looks like, and explain the three types of information you can get from each peak.

II. Distinguishing Equivalent H's

1. Explain what it means for hydrogen atoms to be equivalent or non-equivalent.
2. Describe the rules by which you can determine whether 2 H's are equivalent.
3. Determine the number of sets of equivalent H's in a compound, and circle them on the line structure of the compound.

III. Chemical Shift

1. Describe the chemical shift axis on an NMR spectrum, including where 0 is located, what the units are, and which direction is indicated by the terms “upfield” and “downfield.”
2. Explain why a reference compound is used, and why tetramethylsilane (TMS) is a good reference compound.
3. List 5 rules you can use to predict the relative chemical shift of two sets of equivalent H's.
4. Predict the relative chemical shifts of two sets of equivalent H's.
5. Explain why some peaks which are not equivalent can overlap, and predict sets of H's whose peaks are likely to overlap.
6. Use a list of common chemical shift ranges to predict the range of H's in various functional groups.
7. Predict the chemical shift order of all sets of equivalent H's in a compound.

IV. Integration

1. Explain what integration is and what it tells you about a peak.
2. Predict the integration ratio for a compound.

3. Explain how to measure the integration on a spectrum.
4. Match the predicted integration of a compound with the integration of peaks on a spectrum.
5. Sketch the integration of a known compound on its spectrum.
4. Give a reasonable integration for the spectrum of an unknown compound.

V. Spin-spin splitting

1. Explain what splitting means, and what it tells you about a peak.
2. Explain the $n + 1$ rule for determining the splitting of a set of H's in a compound.
3. Sketch a doublet, triplet, quartet, quintet, and multiplets with correct relative heights.
4. Predict the expected splitting for all peaks in a compound.
5. Explain what happened when two peaks overlap to form a complicated multiplet.
6. Explain why complex splitting can occur when coupling constants are not the same.
7. Explain what usually happens with the splitting in OH and NH peaks, and how this can change if the sample is very dilute and dry.

VI. Deuterium in NMR

1. Explain what deuterium is and why it is useful in NMR.
2. Explain what two deuterated solvents are commonly used in NMR, what kinds of compounds they are used with, and where their solvent peaks show up.
3. Explain where water will show up on an NMR spectrum.
4. Explain what happens when D₂O is added to a spectrum containing an alcohol, amine, carboxylic acid, or amide.

VII. Carbon-13 NMR

1. Explain why ¹³C NMR is less useful than ¹H NMR.
2. Explain what you will see in proton coupled and decoupled spectra.
3. Explain what the most common use of ¹³C NMR is.

4. Predict the number and general location of peaks in the ^{13}C spectrum for a compound using a table of chemical shifts.

VIII. Practice with NMR spectra

1. For a given compound, make a chart giving the expected integration, splitting, and chemical shifts for each peak.
2. Match the H's in a compound with the peaks on a spectrum using the expected integration, splitting, and chemical shifts.
3. Use the chart to sketch a spectrum showing the approximate chemical shifts, expected splitting (with no overlapping), and the integration line.
4. Analyze the integration, splitting, and chemical shifts of a spectrum to deduce the structure of a compound matching a given molecular formula.