

5.S: Structure Determination (Summary)

Before moving on to the next chapter, you should:

- Be able to identify groups of chemically equivalent protons and carbon atoms in a structure.
- Be able to explain the basis of an NMR experiment in terms of the spin state of a nucleus, the ground state to excited state transition involved, and the frequency of radiation absorbed.
- Understand the differences between proton and carbon NMR experiments, and explain why carbon spectra generally have more noise, do not show coupling, and do not suffer from the disadvantage of overlapping peaks. You should be able to explain why $^{13}\text{C} - \text{NMR}$ peaks are not usually integrated.
- Understand how to look at an NMR spectrum, including the meaning of the ppm label on the x-axis, the meaning of 'chemical shift', and the definition of zero ppm on the chemical shift scale.
- Be able to predict trends in chemical shifts for protons and carbon atoms in different bonding positions, and provide a rationale for the trend. You should also be able to roughly estimate the chemical shift of a given proton or carbon using Table X or a similar table from another source.
- Understand how to use proton peak integration values to determine how many protons a particular peak is 'worth'.
- Be able to explain the physical basis for spin-spin coupling in $^1\text{H} - \text{NMR}$ spectra, and be able to use the 'n+1 rule'.
- Be able to interpret, and draw splitting diagrams for, $^1\text{H} - \text{NMR}$ spectra with complex coupling.
- Be able to use a $^{13}\text{C} - \text{NMR}$ spectrum to identify the number of magnetically nonequivalent types of carbon in an unknown compound.”
- Be confident at working problems in which you are asked to match structures to ^1H - and/or $^{13}\text{C} - \text{NMR}$ spectra.
- Given a molecular formula (or a combination of combustion and MS data), you should be confident in your ability to solve an unknown structure based on a ^1H - spectrum, possibly in combination with data from $^{13}\text{C} - \text{NMR}$, IR, or UV-Vis spectroscopy.

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