CHAPTER OVERVIEW

5: Structure Determination II - Nuclear Magnetic Resonance Spectroscopy

In the previous chapter, we learned about three important analytical techniques which allow us to deduce information about the structure of an organic molecule. In IR spectroscopy, transitions in the vibrational states of covalent bonds lead to the absorbance of specific infrared frequencies, telling us about the presence or absence of functional groups in the molecule of interest. In UV-Vis spectroscopy, transitions in the energy levels of electrons in pi bonds lead to the absorbance of ultraviolet and visible light, providing us with information about the arrangement of double bonds in a molecule. And in mass spectrometry, we are usually able to learn the molecular weight of a sample molecule, in addition to other kinds of information from analysis of the masses of molecular fragments.

Although all three of these techniques provide us with valuable information about a molecule of interest, in most cases they do not – even in combination – tell us what we, as organic chemists, most want to know about our molecule. Specifically, these techniques do not allow us to determine its overall molecular structure – the framework, in other words, of its carbon-carbon and carbon-hydrogen bonds. It is this information that we need to have in order to be able to draw a Lewis structure of our molecule, and it is this information that is provided by an immensely powerful analytical technique called nuclear magnetic resonance (NMR) spectroscopy.

In NMR, the nuclei of hydrogen, carbon, and other important elements undergo transitions in their magnetic states, leading to the absorbance of radiation in the radio frequency range of the electromagnetic spectrum. By analyzing the signals from these transitions, we learn about the chemical environment that each atom inhabits, including information about the presence of neighboring atoms. In this chapter, we will see how information from NMR, especially when combined with data from IR, UV-Vis, and MS experiments, can make it possible for us to form a complete picture of the atom-to-atom framework of an organic molecule.