6.S: Summary

Concepts & Vocabulary

6.2 C-13 NMR Spectroscopy- Signal Averaging and FT-NMR

- The magnetic moment of a ^{13}C nucleus is much weaker than that of a proton. This means that NMR signals from ^{13}C nuclei are inherently much weaker than proton signals, which makes ^{13}C NMR harder to acquire good data.
- Chemical shift is similar to ^1H, where the environment around the carbon changes for each carbon in the molecule.
- Integration is not done in ^{13}C NMR spectroscopy because the signals for some types of carbons are inherently weaker than for other types.
- Because of the low natural abundance of ^{13}C nuclei, it is very unlikely to find two ^{13}C atoms near each other in the same molecule, which means that spin-spin coupling is not observed between neighboring carbons in a ^{13}C NMR spectrum.
- There is heteronuclear coupling between ^{13}C carbons and the hydrogens to which they are bound, proton-coupled ^{13}C spectra show complex overlapping multiplets, which makes for a very difficult interpretation. For clarity, broadband decoupling is used, which essentially 'turns off' C-H coupling, resulting in a spectrum where all carbon signals are singlets.

6.3 Characteristics of C-13 NMR Spectroscopy

- Carbons resonate from 0-220 ppm relative to the TMS standard, as opposed to only 0-12 ppm for protons. Because of this, ^{13}C signals rarely overlap, meaning we can almost always distinguish separate peaks for each carbon.
- The ^{13}C NMR is used for determining functional groups based on characteristic shift values.
- ^{13}C chemical shifts are greatly affected by electronegative effects and magnetic anisotropy.

6.4 DEPT C-13 NMR Spectroscopy

- Distortionless enhancement by polarization transfer, DEPT, is one of these techniques and making it possible to distinguish between methyl (CH_3), methylene (CH_2), methine (CH), and quaternary carbons.
- In DEPT, it takes advantage of the ^{13}C to ^1H coupling that is removed in broadband-decoupled ^{13}C spectra.

6.5 Interpreting C-13 NMR Spectra

- Chemical shift is a big indicator into what type of carbon is at that resonance.
- Different carbons are carbons in distinct chemical environments and each different carbon will appear at a different resonance.
- Tables of chemical shift data can be used to distinguish different types of carbons.

6.6 Uses of ^{13}C NMR Spectroscopy

- ^{13}C NMR spectroscopy derives information that is helpful for structure determination.
- Scientists use ^{13}C as a way to determine how many non-equivalent carbons are in a molecule of interest.

Skills to Master

- Skill 6.1 Distinguish between different types of carbons in a molecule.
- Skill 6.2 Estimate the chemical shift of carbons.
- Skill 6.3 Know which carbons will be more downfield.
- Skill 6.4 Determine which carbons are attached to hydrogens using DEPT
- Skill 6.5 Solve unknown structure determination problems with ^1H and ^{13}C NMR spectroscopy.