

Homework #2

Due: 2/1/16 by 5PM...in the "box"

Read: Pages 491- 493 (12.1 and 12.2) and Chapter 13

Do problems: 13.1, 13.2, 13.3b&d; 13.4, 13.5, 13.6 (sketch the predicted spectra), 13.9 a,b,c&d; 13.10.

Supplemental problems:

1. The resonance frequency for ^1H at 4.7 Tesla is 200 MHz. What magnetic field strength is required to create a 400 MHz proton nmr spectrometer?
2. Your new proton nmr machine has a spectrometer frequency of 900MHz for protons. This is nearly as good as they get! Your old 300MHz nmr was barely able to resolve peaks that differ in chemical shift by 0.25 ppm. What is the difference in frequency (in Hz) between peaks at 1ppm and 1.25ppm on the 300MHz machine and what is the difference between these same peaks (in Hz) on the 900MHz spectrometer?
3. Please sketch the nmr spectrum of 2,2,5,5-tetrachlorohexane ($\text{CH}_3\text{CCl}_2\text{CH}_2\text{CH}_2\text{CCl}_2\text{CH}_3$). Your sketch should include the relative position of all peaks and integrals of these peaks. The absolute chemical shifts are not important in this problem, only the relative positions.
4. A valuable unknown has an empirical formula of C_4H_9 . The compound has a single high field peak in the ^1H nmr and a molecular ion at $M/Z = 114$. Please propose a structure for the unknown molecule and predict the M/Z of the most intense fragment you expect to see in the mass spectrum for your unknown.