Go to http://www.nd.edu/~smithgrp/structure/workbook.html and solve problems 1, 2, 3, 14, 19, 27, and 28. In each case, take a good look at the IR, H1 NMR, and C13 NMR spectra. Draw a clear structure indicating every H atom, with designations clearly indicating splitting (s for a singlet, d for a doublet, t for a triplet, q for a quartet, beyond that just m for “multiplet”) and chemical shift (δ ppm) for the 1H spectrum. Explain the splitting patterns and say just a little about why the peaks appear in the vicinity of the chemical shift you indicate. For example,

![Structure](image)

The CH₃ groups are singlets because they have no other CH groups near them; they appear around 2 ppm because they are next to a C=O group. They are at the same chemical shift because they are in equivalent environments.

Support your assignment by mentioning at least two features of the C13 spectrum and two features of the IR spectrum that support your assignment.

NOTE: Be on the alert for situations where two hydrogen atoms are on the same carbon but are in DIFFERENT magnetic environments. Examples of this sort of situation are given below. Note that when this is the case, the H atoms will probably have different chemical shifts and will also split each other’s peaks. Their splitting patterns may be quite complex. Don’t worry about explaining these complex patterns; just be on the alert for them and call them “multiplets.”

![Diagram](image)

Additional comments:

1H spectra: At this site, if you click on a peak, you may get an expanded version.
Carbon-13 spectra: The lines around 77 ppm are due to CDCl₃. They can be ignored. Note that the mass spectrum is also there. It can sometimes be helpful. Some of the peaks in the C-13 spectra are marked with s, d, t, or q. This indicates the results of an “off-resonance” experiment, where the number of H atoms attached to the C atom is determined. s means a C with no hydrogens attached, d means CH, t indicates a CH₂, and q indicates a CH₃.