Distortionless Enhanced Polarization Transfer Spectra

Answer these questions on your spectra, if possible. No additional sheets are necessary.

What is you (un)known number and compound?

How many different carbons are present? (from the number of peaks in the C-13 spectrum) How many carbons are associated with each peak? (from the height of the peaks) How many attached hydrogen atoms are there on that carbon?

Attach the decoupled C-13 spectrum (the "normal" C-13 spectrum) and the DEPT spectra. Label the peaks A, B, etc. corresponding to your answer above.

Draw the structure of the known alcohol, give its name, and label the carbons in the structure so that they correspond to the table above.

DEPT Spectra

DEPT (distortionless enhanced polarization transfer) spectra are series of three C-13 NMR spectra that are usually arranged from bottom to top as follows:

The bottom spectrum is a normal, decoupled C-13 NMR spectrum.

The middle spectrum (DEPT-90) shows all carbons with exactly one hydrogen atom attached to them. These carbons are called tertiary.

The top spectrum (DEPT-135) shows carbons with odd numbers of hydrogen atoms (primary and tertiary carbons) as up peaks and even numbers of hydrogen atoms with down peaks (secondary carbons.

The DEPT-90 and DEPT-135 spectra are collected in a way that is similar to a normal C-13 spectrum. As you saw in the first lecture, the normal spectrum is collected by applying a pulse of energy covering a range of frequencies to your sample with the ^{1}H decoupler turned on and then measuring the sample's response to the absorption of that energy. The DEPT spectra differ in that more than one pulse is applied (both ^{13}C and ^{1}H) before measuring the sample's response. This will be covered in greater detail at the end of the course.

Interpretation of the DEPT spectra then allows you to assign each peak in the spectrum to a carbon with no hydrogen atoms (quaternary), one hydrogen (methine), two hydrogen atoms (methylene) or three hydrogen atoms (methyl). Briefly, a quaternary carbon will appear on the normal (bottom) spectrum, but no others. It will be unusually short. Methines (tertiary carbons) appear on the DEPT-90 (and both other spectra). Methylenes (secondary carbons) appear as down peaks on the DEPT-135 and methyls (primary carbons) appear on the normal spectrum and DEPT-135, but not the DEPT-90.

Solve the following structures from their C-13 spectra:

Molecular Formula	chemical shifts (DEPT results, intensity) u = up peak, n = no peak, d = down peak Three results from bottom to top on DEPT spectra.
a) C_4H_9Br	12 (unu,1), 26 (unu,1), 34 (und,1), 53 (uuu,1)
b) $C_5H_{11}Cl$	9.5 (unu,1), 32 (unu,2), 39 (und,1), 71 (unn,1?)
c) $C_5H_{11}Cl$	22 (unu,2), 26 (uuu,1), 42 (und,1), 43 (und,1)
d) C_9H_{12}	24 (unu,2), 34 (uuu,1), 126 (uuu,1), 126.5 (uuu,2), 128 (uuu,2), 149 (unn,1?)
f) $C_4H_8O_2$	19 (unu,2), 34 (uuu,1), 184 (unn,1?)
g) $C_4H_8O_2$	22 (unu,2), 67 (uuu,1), 161 (uuu,1)